Computer Support for Conceptual Process Design

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MPhil

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1997

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Abstract

Since the introduction of computers into the field of chemical engineering in the late 1950s there has been a rapid expansion in their use to the point that they are currently considered to be an essential tool of daily working. The majority of users utilise their available computing power in a relatively low level way to carry out mathematical calculations. This usage pattern has lead to a profusion of stand alone computer based tools, such as flowsheet simulators, each information hungary and capable of producing large quantities of data. Rather than being a slave to complex, and often tedious, manual calculations the process engineer runs the risk of being swamped by data handling requirements and confused by the range of available tools. One of the challenges facing those working to improve the computer aided design process is to seek ways to employ the capabilities of computers more effectively. An essential prerequisite to this is developing a realistic model of the design process.

After considering the history of the use of computers in Chemical Engineering this thesis reports a market survey of a broad spectrum of process industry companies. The survey is used to gain knowledge of the computer based design facilities used by the companies and to develop an understanding of the facilities that they would like to have at their disposal. This information obtained is then used to help ensure the wide scale acceptability of any tools developed. Before examining the application of novel design aids the suitability of existing models of the design process as a basis for tool development is examined. A hierarchical model is found to be most appropriate. The shortcomings of the most prevalent hierarchical model, due to Douglas, are discussed and any alternative form presented to overcome these. Three tools developed in the Department of Chemical Engineering at the University of Edinburgh are utilised using a case study approach. CHiPS is a whole plant process synthesis tool with somewhat limited utility due to the restricted number of unit operation models available. KBDS is a computer based design support tool with group working capabilities. A prime advantage of using KBDS is the ability to record an auditable design history trail. Épée is an object oriented process engineering environment which integrates design tools and allows information to be passed between them without being rekeyed by the user. The integrated environment approach helps ease the data handling burden on the user and minimises the possibility of errors. To ensure that inherent safety is included in a design a modified hierarchical approach to hazard studies is proposed. This builds on earlier work undertaken at Edinburgh.

Frontispiece

This thesis is dedicated to those who helped me in the long struggle for completion.

To my husband, Ian Woodcock, for moral and financial support.

To Geoff Ballinger, Helen Denton, Colm Fitgerald, Don and Liz Glass, Lesley and Tarig Musa, Mairi Simpson and Jennifer and Neil Skilling for putting me up and feeding me during my visits to Edinburgh.

"The best computer in the world is of no value to the chemical engineer unless he can understand his own problem, formulate it and devise a method of solution."

Jenson and Jeffreys

"Elimination from accumulation is the process of finding what you want."

Charlie Chaplin

The work described in this thesis is the original work of the author and was carried out without the assistance of others, except where explicit credit is given in the text. It has not been submitted, in whole or in part, for any other degree at any other university.

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Chapter 1

Introduction

The work described in this thesis is concerned with the use of computers to support the design of chemical process plant, with a particular emphasis on the initial, or conceptual, phases of design. The aim is to establish how this phase can best be supported in order to improve the quality of the designed product with respect to the factors necessary to achieve a successful project.

In order to use computers in the most suitable way for this role it is necessary to develop an understanding of *who* undertakes process design, *why* they do it and *how* they do it, as well as being familiar with the capabilities and limitations of hardware and software. This understanding then forms the platform upon which to build appropriate tools. Chapters 2 and 3 describe work to develop this understanding. Chapter 2 looks at the history of the use of computers in chemical engineering whilst Chapter 3 explores the user based questions via a market survey. Modifications of existing methods to improve the design quality are explored in Chapters 4 and 8 which focus on design methodology and hazard studies respectively. The use of tools proposed to support the design process is discussed in Chapters 5, 6, and 7 via their application to a case study. Conclusions are drawn in Chapter 9 and a glossary is included in Chapter 10.

Sections 1.1, 1.2, 1.3 and 1.4 define the motivations, starting points, phases and measures of success used as a basis for this work.

1.1 Motivation for Design.

Designs of any type do not simply happen they occur because there is need for the end product of the design process. At the most fundamental level the products of design are needed to satisfy the basic human needs of water, food and shelter, and as such the motivation is the desire to survive. However when considering process design the needs that the product of design will satisfy have moved far beyond the basic human needs and the motivation for undertaking the design process has become much more complex.

Imagining the motivation for design at the two extremes of possible economic market models defines the bounds for the situation that will actually exist for most projects. In a situation that is purely driven by market forces with no constraints applied then the motivation would always be to maximise the amount of money that could be generated. Conversely when the market is subject to constraints that ensure resources are allocated and used in such a way that maximises the benefit to all members of the society then the motivation will be to increase the general well being. In reality neither of these extremes actually occurs with the actual motivation being supplied by the starting point for the design applicable in the case under consideration. This is discussed further below. At the individual level it is unlikely that a process engineer will spend a significant amount of time analysing the motivation to carry out design as there is no method for engineers analogous to the method acting technique favoured by some in Hollywood (Miller 1987). For them design is carried out because it is their job.

1.2 Starting Points for the Design Process.

Not all process designs will start at the same point due to differences in factors such as state of technology and information available. The history of a design will depend on the starting point for that design and as such it could be said that a different model of the design process would be necessary for each possible starting point. However, at best, this approach would result in a cumbersome structure of models but it is more likely that the a different model would be required for each design making the approach completely unworkable. An alternative approach is to develop a general model of the design process which allows entry at different levels depending on the starting point. The cases given below represent the range of entry points that can occur, starting with the most abstract and moving down to the most tightly defined. Entry points at the top of the range occur for projects that require considerable pre-definition, and hence exhibit the greatest opportunity for the design process to influence the designed object. At the bottom of the scale the project is largely predefined and there are few degrees of freedom in the design.

Case 1 Want to produce a material with specific physical or chemical properties in order to fill a perceived gap in the market.

Case 2 Believe that a new, more beneficial, route to an existing product can be developed.

Case 3 Have a quantity of material produced as a by-product or waste from an existing plant that may be capable of use to produce a valuable product.

Case 4 A new product, which would be in direct competition with existing materials, is to be introduced onto the market.

Case 5 Need to install a derivatives or feedstock plant, using existing technology.

Case 6 An existing plant has reached the end of its' life and is to be replaced with a new plant using the same technology.

Case 7 By making major modifications the capacity of an existing plant can be significantly increased.

Case 8 Minor modifications will result in debottlenecking and improve the operation of the plant.

A generally applicable model of design must be able to accommodate the full range of entry points.

1.3 Phases of Design.

All designs originate as an abstract idea that must be subject to development before the physical realisation of the design can be achieved. This principle applies to tasks that occur in everyday life, such as the installation of a bathroom, as well as to more commonly accepted applications of a design process, such as the installation of a new oil refinery. In the case of process plant design the completion of the design phases does not mark the end of the life of a project as it then passes to construction, commissioning and operation, mirrored by installation and use in the bathroom example. After a number of years in operation, during which modifications will be continually performed, the process plant will be decommissioned, which marks the final completion of the project that started with an abstract idea. Even at this stage individual items of equipment may be reused on other projects in alternative duties. With the bathroom example modifications are less likely to occur during the lifetime of the installation with decommissioning

occurring when a more fashionable version is installed. In either case the lifetime of the project can reach 30 years or more.

Scott and Crawley split a project into four stages with the ideal situation being that each be completed and reviewed before the next is commenced, the likelihood of overlap is emphasised (Scott and Crawley 1992). The four stages are:

(i) Conceptual Design. Where the fundamental questions such as plant capacity, chemical route, plant location and basic economic viability are addressed.

(ii) Detailed Design. Where the bulk of the design takes place to result in a complete specification of the plant.

(iii) Construction and Commissioning. The physical realisation of the plant is built and then process materials introduced to bring it into operation.

(iv) Operation and Maintenance. Hopefully the longest of the stages with the plant undergoing modifications and well as the maintenance routines necessary to keep it running.

Other varying structures for this purpose often involve more stages. In the break down of a project, from a project engineers point of view rather than that of a designer eight steps are identified, (Rose et al 1978), each having a number of possible subdivisions. The eight steps are:

(i) Project preliminaries

(ii) Process design

(iii) Basic engineering design

(iv) Detailed engineering design

(v) Procurement

(vi) Construction

(vii) Commissioning

(viii) Production

The subdivisions occur during the early phases with project preliminaries having two and process design four. These are linked in with the need to provide a relatively large number of estimates during the early phases of the design to allow

the project to progress through the various sanction stages, where the money necessary to fund further development are made available.

The examples given above highlight the two possible approaches to defining the phases of design. In the first case the evolutionary gap between the stages are large and the emphasis is on significant changes in the activities being undertaken. Another view is taken in the second case were a shift in emphasis focuses attention on divisions that arise due to project management considerations. Neither of these two structures is entirely appropriate for the purposes of the work being discussed here and the phases listed below will be used. These are based on the authors own experience of a range of process designs and cover the full life of a project rather than simply the design phases.

(i) Feasibility Studies. This is a rather abstract stage at which the impact of sweeping changes in project parameters, such as processing schemes, location and capacity, are investigated. The low level of detail involved allows a relatively large number of options to be considered and an overview of alternative strategies to be prepared.

(ii) Conceptual Design. This is the stage at which process design work begins in earnest. A number of important project factors, such as route details, may still be undefined leading to the study of a small number of options in greater detail than in phase 1.

(iii) Front End Design. Work carried out on a single route in a fixed location to help define the secondary factors and define a front end package that is used as a basis for phase 4. This is where the majority of the process design work is carried out and marks the start of the involvement of other disciplines. P&IDs are produced.

(iv) Detailed Design. The bulk of the process design work will be completed prior to the start of this stage although continued chemical engineering input is necessary to assess the impact of any changes on the design carried out previously. During this phase all the details necessary to allow the plant to be built are defined and the appropriate items of equipment ordered. A large multi-disciplined task force is assembled to add detail to the process design package. At this point all the material necessary to construct the plant are

purchased making procurement an integral part of the phase. The tie is strengthened by the need to incorporate vendors information into the design.

(v) Construction and Commissioning. Covers the period from the start of the first construction contract, likely to be site preparation, to the start of beneficial operation. In addition to building the plant trials must be carried out and operators trained. Such activities overlap to such an extent that separation of the two activities is difficult.

(vi) Operation. Covers the bulk of the life of a project from the point at which beneficial operation is established to decommissioning. During this period the plant will be maintained to keep it in a state fit for operation and modifications will take place. These will range in complexity and requirement for design input from changes in operating practises to rebuilds.

(vii) Decommissioning. The plant reaches the end of it's useful working life and is taken out of service. Demolition will occur at some point with elements of the plant being reused if suitable.

The phases involved in a design will be dependant on the particular project being undertaken, although the latter phases will be common to all plants that are actually built and run. Common variations on the phase structure would be, for well defined projects, phases 1 and 2 combined and the splitting of phase 5 into separate construction and commissioning phases. This structure is discussed by (Chambers 1994) when looking at a large chemical industry project.

1.4 Measures of success in Design.

How successful a particular design is judged to be depends very much on the current viewpoint of the person asked to make the judgement as measures of success are highly subjective. As well as varying between individuals, or groups of individuals with the same perspective, whether or not a project is assessed as being a success or a failure depends on the point at which the judgement is being made and the external conditions that prevail at the time. Consider a project which encounters difficulties during the design phase causing budgets and schedules to be exceeded but then runs smoothly and profitably for longer than the design life. Viewed with an

accountancy or project management outlook during the design phase the verdict would be one of failure but this would be reversed if the opinion of plant management were sought after 20 years of operation. There have also been many examples of processes designed and run to produce materials later found to have such significant SHE impact to cause the subsequent banning of either the method of manufacture or any production. Recent examples in this category are the moves away from CFC refrigerants and from leaded fuel both of which were highly successful at fulfilling their respective roles until the impact on the environment was discovered. The more environmentally friendly replacements are less successful in fulfilling the basic function. Whilst these examples highlight the fact that a full assessment of a project can only be made towards, or ideally at, the end of its life span, it must be realised that for a project to pass through all the phases mentioned in section 1.3 then judgements of the probability of overall success, based on incomplete information and conjecture, must be made at the conclusion of each phase. These judgements determine if a project will proceed to the next stage or be abandoned, and it is obviously essential that every effort is made to ensure that the basis is as accurate as possible and that all the relevant factors have been considered. A decision to stop a project becomes increasingly difficult and complex as the number of stages completed increases, due to the expenditure of effort and time as well as money, involved in reaching the latter phases. For this reason it is unusual, but not unknown, to see projects that are stopped after detailed design when equipment starts to arrive on site for construction. An example of such a project is the Occidental refinery on Canvey Island in Essex, which was halted after construction had started and the bulk of the equipment had been purchased. This occurred in the mid 1970's when the oil crisis caused a dramatic shift in the economic case for the refinery so that it became untenable to proceed to plant operation. To allow for extreme changes, occurring over a short time period, in the factors used during project evaluation would be outwith the capabilities of standard sensitivity analysis methods employed to account for uncertainty. Another factor that is difficult to pre-empt and that has a significant impact on the long term viability of a project is legislation.

There are six characteristics that can be used as a good general basis for

establishing if a project is a success or a failure and these will be discussed in detail in Chapter 4. Briefly to be judged a success a project must be clean, constructible, cost-effective, maintainable, operable and safe. Which combination of these characteristics is used during project assessment to determine the likelihood of success is dependant on the stage which the project has reached with constructability and maintainability appearing at a later stage than the others.

Chapter 2

The Use of Computers in Chemical Engineering

2.1 Introduction of Computers into Chemical Engineering.

Chemical plants have been successfully designed, built and run on a large scale since the industrial revolution and the process predates the wide scale use of computers by more than a century. The relatively short history of the use of computers in chemical engineering is illustrated by the fact that the European Federation of Chemical Engineering (EFCE) first established a working party on this topic in 1966. This working party was responsible for setting up and organising a series of symposia on Computer Applications in Chemical Engineering (CACE) the twelfth of which was held in 1979. A review of early work in this field undertaken at CAD Centre, Cambridge, is given by (Leesley 1973). Four tools available commercially at that time are described: SYMBOL was a mass balance tool for use during the early stages of design, CONCEPT a simulation tool, ASME 8 addressed the design of pressure vessels and PIPER was for piping system design. In a review of work and a look forward to the future published in 1980 Evans refers to process flowsheeting, (Evans 1980). This terminology has now largely been superseded when referring to computer tools other than those involved with the mechanism of drafting PFDs. Current terminology refers to the function of the tools to be used, eg simulation and synthesis.

Whilst the era when computers were seen as an expensive luxury rather than as an essential design tools has long since passed, for many designers restrictions in access to suitable facilities still prevents the level of usage envisaged by many people involved in the development of design tools. In his IChemE jubilee plenary lecture in 1982, Sargent stated that software was available for every kind of design calculation and implied that graphics packages were sufficiently advanced to signal the demise of the engineering draughtsman, (Sargent 1982). Viewed from fourteen years later these statements still seem over optimistic as hand calculations are still routinely carried out and draughtsman, in reduced numbers and using CAD not boards and paper, are an essential part of any design office.

Exaggerated claims of the capabilities of computing systems and the advantages that can be gained by their use that are not borne out in practise, such as these, have contributed to the slow acceptance of the "new" technology. Berzins and Jones highlight this point in their discussion of process engineering databases where disappointment in the performance of first generation systems resulted in a greater reluctance to invest the time, money and effort needed to adopt improved second generation systems, (Berzins and Jones 1989). This point is further reinforced by Reese who, when discussing Chevron's experience with real-time control and process information systems, states that poor management experience of early systems caused a twelve year gap, between 1965 and 1977, where no projects were attempted, (Reese 1989). Such reactions are part of human nature on the level of "once bitten, twice shy" but ignores the valuable learning experience that can be gained by getting things wrong. The need to demonstrate actual practical advantages of techniques and tools before they are generally accepted can be illustrated by considering the history of plant models.

Today the term plant modelling has become synonymous with the use of computers for the running of a series of mathematical models representing the unit operations and equipment items making up a chemical plant. However this is a relatively modern usage that has developed hand-in-hand with the use of computers in process design. The original meaning of this phase related to the building and use of scale models of a plant during the design phase. Even with the advent of 3D CAD, enabling walk through models to be realised, such scale models are sometimes still built. In the light of such advances the initial impact of such models on process design is difficult to envisage but never the less during the late 1940's and early 1950's they represented the forefront of technology. As pointed out by (Taylor 1995) the plant models could be used to allow faults in design, such as valves that could not be reached, to be spotted at a sufficiently early stage in design to be rectified at a minimum cost. Models are also a "user-friendly" way of presenting a large quantity of data to people with a wide range of experience. This is one of the main reasons for their continuing use in the face of their relatively high production costs. They also look impressive sitting in the foyers of corporate headquarters. As with any innovation in design the use of scale models was slow to be adopted by

main stream engineering firms with wide scale use only following practical demonstrations that the tools could bring improvements in design quality without imposing a significant financial burden (Taylor 1995).

Since the hurdle of wide spread acceptance of computers as a useful design tool was passed there has been a rapid expansion in the emphasis and reliance placed on their use. Process engineers have been far from slow in realising the potential of computers to aid their calculations, spreadsheets now being widely used for this purpose. A review of their application in chemical engineering is given by (Rosen and Adams 1987) who include a discussion of the limitations of these tools. However, as pointed out by (Ballinger et al 1994), whilst the productivity of process engineers, in terms of the amount of data produced, has undoubtedly benefitted from the introduction of computers it is doubtful if creativity or ease of production have been enhanced. Concerns have been expressed for sometime, (Sargent 1982 and Matzopoulos 1996), that there is a danger, amongst those who have been both educated and employed in an environment with easy access to design tools, of a dependence on the tools developing. If this occurs then the software is treated as a black box, using calculation methods that are not fully understood and producing answers that are not queried. In this situation it is likely that undetected errors will occur due to either the use of an inappropriate method or incorrectly input data. This risk is exacerbated by the difficulties inherent in checking most computer generated calculations. Hanyak and Jannuzzi propose a system, BUTS, to address some of these concerns, (Hanyak and Jannuzzi 1989). BUTS is aimed at allowing students to develop an understanding of the thermodynamic principles involved in a design before moving onto the use of a standard simulator. Grasty developed a relatively simple "sceptic" system to check the mass balance calculations performed by ASPEN, (Grasty 1993). The system analyses the files of a run and uses fundamental principles to check items such as the order of relative volatilities, as well as the mass balance. A report of the magnitude of errors found is then produced. The concept could be extended to cover heat balances. Mass and heat balances are key to the overall manual checks that would be performed on a design, but at the equipment level checks are type dependant. eg for a heat exchanger temperature approaches and pressure drops would be looked at but for flash vessels vapour space height and

liquid level would be checked. Such variation would make a "sceptic" system for equipment size and duty checking more complex than one for checking balances.

Matzopoulos points out that the dependence on commercial software is encouraged by moves towards tools, particularly simulators provided by companies such as Hyprotech and Aspen Technology, which provide the GUIs and model libraries that allow users to build working simulators quickly, easily and, perhaps, without fully understanding the problem that they are trying to solve, (Matzopoulos 1996). An alternative approach to the use of such software packages is to consider the use of a generalised equation solver such as gPROMS. Design using this type of tool requires the user to have a high level of understanding of the process and to possess considerable mathematical skills. Those undertaking design are highly unlikely to have the luxury of the time that using this type of tool entails, hence the popularity, see Chapter 3, of the first type of tool. Indeed, the ability of users to produce seemingly meaningful work from a tool shortly after starting to use it is seen as a strong selling point which is highlighted in sales literature such as that produced by Cherwell Scientific to support the launch of PROCEDE v2.1, (Cherwell 1995). Whilst some companies are concerned that using commercially available tools will lose them the competitive edge, (Matzopoulos 1996), few can afford to maintain the teams of people necessary to develop and serve in-house simulation tools. An example of this is the recent move by ICI to stop supporting their own in-house simulator and buy into industry standard tools. Evans quotes a typical development effort of 20 to 60 man years spread over 3 to 5 years at a cost of several US million dollars for a working flowsheeting tool, (Evans 1980).

Given the relatively short period over which computers have been used to undertake design calculations, the advances made have been impressive and the rate of change rapid. As this situation is likely to continue for sometime, with the next technological advance being difficult to predict, it is important to consider upward migration during the development of tools, (Preece and Stephens 1989). Evans summarised the situation with respect to the use of computers in design in 1980 as follows:

(i) Tools commonly used at that time performed steady-state simulation, equipment sizing, cost estimation and project economic evaluation.

(ii) Areas identified as being up and coming were dynamic simulation, optimization, synthesis, scheduling of batch operations, energy efficiency analysis, safety and reliability analysis and probabilistic flowsheeting.

With the benefit of hindsight the future areas identified, with the exception of the last, have all had a substantial amount of effort devoted to them in the intervening years. The degree of success in developing useable tools is, however, highly variable.

One aspect that has remained essentially unchanged as the acceptance of, and possibly reliance on, computers has increased is the way in which computers are used. They are generally viewed as a means of undertaking numerical manipulations. The potential for utilising and organising the vast quantities of data that can be produced, via integrated DBMS or similar facilities, has not yet been fully exploited. Additionally, techniques developed in the field of artificial intelligence for the manipulation of non-numeric knowledge offers potential benefits that have not been explored. A review of artificial intelligence in process engineering is given by (Stephanopoulos 1990). Stephanopoulos highlights the draw-backs of focusing on numerical computations alone as being the inability to record design history, failure to support conceptual development, the possibility of over loading the user with so much information that the important elements are swamped, reliance on assumed values of parameters, inability to adequately support planning and scheduling and limited control system performance analysis. The key to the application of AI in engineering is the modelling of knowledge. Refer to Chapter 4 for a discussion of the modelling of the design process.

2.2 Development of Hardware.

The general acceptance and use of computers has followed the development of hardware that is both reliable, affordable and accessible. Motard estimated that between 1955 and 1985 the cost of computer hardware had dropped by a million fold, (Motard 1983). It is usual to refer to computers as belonging to one of five generations linked with the technology used in their construction. These five generations are defined as follows, (Chandor et al 1985):

First Generation - Constructed using thermionic valves.

Second Generation - Built with transistors.

Third Generation - Built with integrated circuits.

Fourth Generation - Computers which use very large scale integration, VLSI, and consist of integrated circuits containing several hundred thousand transistors.

Fifth Generation - A future generation of computers intended to be addressed in natural language and to exhibit artificial intelligence.

Moving down through the generations, not only have the components used in the manufacture of the machines become more robust but there has been a marked reduction in the physical size of a machine required to carry out a given task. This is most clearly illustrated by the move away from large, air-conditioned rooms containing mainframe machines, lovingly tended by a dedicated staff, to PC's and workstations located on the desks of the users. The advent of networks has aided the move away from a reliance on mainframe machines by allowing users access to software mounted away from the machine that they are using and by allowing communication between users.

Today a fairly typical platform used by process designer wishing to undertake reasonably complex design calculations, such as running as simulator and a suite of support programmes, would have the following specification:

Pentium Processor
16MB memory (minimum), 32MB for power users
1.2GB disk space, if standalone with a reduction if networked
Windows '95 or Windows NT

To gauge the development of personnel computing an interesting comparison can be drawn with the system described by Sucksmith, (Sucksmith 1983). For a chemical engineer to undertake design work the features described were: 64 K of RAM, 16 bit microprocessor, monochrome high resolution screen of 25 by 80 character lines, 80 character wide printer, 2 disk drives and a 1200 baud modem. Given such a system and programmes written in Basic, execution times were too

slow to make it possible to run applications as complex as simulators. The most striking advance has been in memory with a 100 fold increase. More sophisticated languages have also been important. Pekny includes an interesting comparison of the hardware that could be purchased for US$2,500 in 1989 and 1994, (Pekny 1994). In 1989 the system comprised of an Intel 80386 CPU running at 20 MHz, 1 MByte RAM and 80 MByte hard disk drive. By 1994 the corresponding figures were 60 MHz, 8 MByte and 540 MByte.

Brulé and Chronister give a brief history of many elements of computing hardware and attempt to identify future trends to aid engineers planning to purchase a system that will not become obsolete too quickly, (Brulé and Chronister 1993). The first PC CPU was Intel Corp.'s 8088 microprocessor, this was a 16 bit device utilising about 1 MB of RAM. This was followed by the 80286 which raised memory capacity to 16 MB. Subsequent generations have been the 80368 and the 486 which is currently being replaced by the 32 bit Pentium. The Pentium can work with a memory of up to 4,294,967,296 bytes. Moving to the use of 64 bit chips with even larger memory capabilities is hampered by the lack of software written to exploit these abilities. Workstation microprocessors are developing along the same lines.

Peripherals have also moved towards an increased storage capacity. The 5.25" floppy, storing up to 1.2 MB, has now been replaced by the 3.5" floppy, storing up to 1.44 MB as the most commonly occurring medium. Other notable advances are towards the use of CD-ROM and DAT units.

One of the latest developments in the search for ever increasing computational power, and hence the ability perform a greater number of numerical manipulations in a given time, is parallel computing. Higher computational rates have the advantage that reduced solution times make it feasible to attempt to solve problems that were previously considered to be too complex. Parallel computing architectures, in principle, involve no upper limit on speed. For process design this allows both more realistic models of unit operations to be tackled and large simulations to be run in a more user friendly way. The speed-up obtained by the application of parallel computing to a plant simulation is dependant on the type of simulator and the choice of an appropriate solution strategy, (Best 1989). Best draws a comparison between

the collection of unit operations that make up a chemical plant and the network of processors within a parallel computer. At a simple level, if a single processor were allocated to each unit operation the network would mirror the physical reality of the plant being modelled. The occurrence of such a mapping between plant and the computer system used to model it was used in the early days of the use of computing in process design as an argument to favour the use of analogue over digital computers, (Rosenbrock and Storey 1966). Haley and Sarma report on an early study undertaken by Du Pont to compare the performance of simulations run on a VAX and a two processor Cray X-MP, (Haley and Sarma 1989). Thirty four test cases based on "real" problems in the chemical process field were run on the two types of machine, twenty eight utilising PROCESS and six the Du Pont in-house simulator, CPES. No attempt was made to alter code to exploit the parallelism of the Cray but the majority of problems ran with a VAX / Cray CPU time ratio of 5 to 6. Haley and Sarma concluded that the Cray was a cost effective way of carrying out process simulations. Harrison explored the use of a utility programme to modify FLOWTRAN coding and allow it to be run on a 2 processor parallel computer, the Cray XMP/24, (Harrison 1990). Such an approach avoids the need for time consuming manual modification of the code. Even given the small number of processors used the utility programme successfully introduced the necessary modifications to achieve some speed-up. It did however miss some opportunities for parallel operations, based on parallel unit operations, that would seem obvious when undertaking manual analysis. Harrison cites the amount of time spent on low-level physical property routines, 50 to 65 % of execution time, as being a significant reason for the lower than expected speed-up. Best also reports on case studies for exploiting parallelism in process design calculations and gives a brief introduction to the hardware and models of parallelism, (Best 1990). He worked with systems based on transputer architecture using algorithmic parallelism as a method of solution. This set-up is best suited to the solution of sequential modular simulation problems. Dualism was used by Best to tackle the problem of the time spent on thermodynamic calculations. To avoid the need for control co-ordination and a potential hold-up in communication all the unit models were designed to proceed as soon as a complete set of inputs become available. As the complete state of the system, in the form of

the steady-state simulation results, is known before a dynamic simulation, full use of co current capabilities can be made to maximise the speed-up seen. The test study results reported by Best bear this out. Four example problems were run using the system proposed by Best and PROCESS as a comparison. Processor topology and communication between processors were identified as key in establishing the speed-up over conventional calculation methods.

O'Neill and co workers examine solution strategies to achieve the best results when applying parallel computing to multicomponent separation problems, (O'Neill et al 1994). They focus on the use of methods exploiting equation based solutions to process flowsheeting as these are claimed to have the greatest potential for exploiting parallel computing. The degree of speed up obtained from the use of parallel computing is related to the degree of parallelisation in the code by Amdahl's law, (O'Neill et al 1994). This states:

$$S_A = \frac{P}{[P(1-f)+f]}$$

Where S_A is the speed up, P the number of processors and f the fraction of the code performed in parallel. Approaches based on the utilisation of sequential modular base codes, such as those due to Harrison and Best, allow maximum use to be made of existing code but limit the parallelisation that can be achieved and hence the speed up. Solution strategies that allow a higher degree of parallelisation, such as that proposed by O'Neill and co workers, increase the speed up achieved. This is partially related to the type of parallelism achievable for the two approaches. In the first case compilers will spot opportunities for low level parallelism but are likely to miss those for high level parallelism. High level parallelism can generally only be exploited by the development of solution algorithms based on knowledge of the type of problem to be tackled. Cera discusses the speed-up obtained for a sequential modular process simulator between a Sun workstation and a BBN Butterfly parallel processor containing sixteen processor nodes, (Cera 1989). A simple double buffering approach is used to decouple the sequential information flow and allow concurrent parallel computation. The simulator used during the comparison was DYFLO running a distillation column model. Distillation was used as a basis as it is commonly occurring and computationally intensive. It also exhibits inherent

parallelism, this was manually identified in the study described. Using 12 processors a 4 fold speed-up was seen for a 10 stage column. With 14 processors and a 50 stage column this rose to 8 fold. The impact of massive parallelism is investigated by Carmichael and co workers who report on the use of a 16,384 processor machine, (Carmichael et al 1989). This was compared to a VAX 11/780 and a Cray-2 for the running of complex models for the prediction of the chemical reactions and transport properties involved with acid rain. Speed-up factors reported were 450 and 10 respectively.

2.3 Development of Software Elements.

To a large extent, particularly for commercially available design tools, the evolution of the software has directly followed, with a lag, the evolution of the enabling hardware. As the cost of the hardware has dropped the software costs, development and maintenance, have become increasingly dominant. There is a large cost induced gap between the hardware platforms used by researchers into the design process who are responsible for the front end development of design tools and those who undertake design on a day-to-day basis who use the ultimately produced tools. This gap is currently illustrated by the fact that most process engineers are currently working with 486 or Pentium PCs on LANs whilst the norm for researchers is a powerful workstation with networking and full Internet access. More advanced hardware such as parallel computers which are far too expensive for commercial use are also being used in fundamental research. The cost of each hardware development drops when it reaches the mass market, therefore those involved in research must, to a certain extent, gamble on the platform that they choose to use as a basis in the hope that by the time any resultant tools are sufficiently developed to reach the market place the necessary hardware will have come within the reach of the target end users. The technology gap inherent in this should not be allowed to act as a barrier to the inclusion of those undertaking design on a day to day basis in the development of design methods. As pointed out by (Sargent 1982) it is not acceptable to entrust the development of design methods entirely to those immersed in computer technology. Collaboration with designers is essential to ensure that the developers understand the requirements of the designers and that the designers

understand what can be feasibly achieved. Features of good software that have been identified are that it should be easy to understand, easy to maintain and modify, and be transportable, (Evans 1980).

2.3.1 Languages

Another important factor driving the development of software tools is the availability of languages in which to write them but as these are largely the province of computer science this factor will not be discussed in detail here. Some of the most commonly used general programming languages over the years have been BASIC, C, FORTRAN and Pascal which are of varying vintage and states of development.

BASIC, Beginners All-purpose Symbolic Instruction Code, is an essentially unstructured and simple to use high-level language that was developed in the mid-1960s as an educational tool, (Gunton 1990). It is best suited to short and uncomplicated calculation routines of the type that are now largely carried out using spreadsheets and is unsuited to large scale simulation tasks. These characteristics make BASIC an effectively dead language with respect to any significant computing applications but due its ease of use it is still supported by most PCs. One additional disadvantage is that there is no standard for the BASIC language, with virtually every manufacturer adopting a slightly different, non cross compatible, version.

FORTRAN, FORmula TRANSlator, is a high-level programming language designed for scientific and mathematical applications that was introduced in 1974, (Gunton 1990). Programming is carried out using a combination of algebraic formulae and English-like statements. As with BASIC it is essentially unstructured and, as pointed out by (Preece and Stephens 1989), is generally unsuited to commercial programme development on microcomputers and workstations. However this language was used extensively in the past for writing many complex calculation procedures, including those used in both steady-state and dynamic simulators, and the investment involved makes it unlikely that FORTRAN will cease to be used in the foreseeable future. One of the major problems with programmes written in FORTRAN code is that they do not easily fit into the modern graphical interfaces, such as Windows based environments, that are expected by users or into data base management systems.

Pascal is also a high-level programming language which was introduced in the 1960s, (Gunton 1990). It is a derivative of ALGOL, ALGOrithmic Language, the first block-structured language, which was introduced in 1958. The advantage that Pascal has over ALGOL is that it can easily be compiled on small computer systems and produces very efficient programs. For these reasons it is one of the languages, along with C, that has been used for major applications development work for MS-DOS. As with most languages, including FORTRAN and C, Pascal is available in a number of versions. The simplicity of PASCAL, which is a well-structured language, enhances the ability to detect programming errors. Motard indicates that languages like PASCAL which encourage the creation of portable and modular programmes represent the way forward for DBMS technology, (Motard 1983b). The US Department of Defence has recognised this and spent time developing a universal system development language, ADA, based on PASCAL.

C is similar to Pascal in that it is a high-level programming language that has a block structure. It possess two features that make it popular for the development of systems software and applications packages for small computers, including PCs. Firstly it produces programs that can easily be moved from one type of computer system to another and secondly, although it is a high-level language, it allows programmes access to low-level functions. As defined by (Gunton 1990) a high-level language is one in which each statement corresponds to a number of machine language instructions. This contrasts to low-level languages, or assembly languages, in which each statement corresponds more or less one-for-one with machine language. Machine language is a programming language that corresponds closely to machine code, the program instructions in the form in which they are executed by a processor, and was introduced in the early days of computing, the mid-1940s. As well as use in the development of MS-DOS applications, mentioned above, C is the major language for the development of UNIX applications. These roles combine to make C the most obvious choice, of the languages mentioned here, for use in the development of design tools to be used in the PC environments that currently dominate. In light of trends in tool development, discussed elsewhere, of particular note here is an enhanced version of C, C++, which supports object-oriented programming.

To service the increased use of artificial intelligence techniques in computing languages such as Prolog and Lisp have been developed. These are both symbol processing languages, (Rogers and Petry 1995). Additionally object processing languages such as C++, Visual Basic and Smalltalk are commonly used for the development of expert systems. Prolog is an inference system with a programme consisting of facts and production rules. This makes Prolog a much smaller language than Lisp, which is a list processing language much used in the USA for artificial intelligence programming. Due to the size of Lisp, considerable computer resources are required to utilise it.

2.3.2 Operating Systems

The first generation of computers had each programme as a stand alone entity but by the mid 1950's it was realised that this was not satisfactory, leading to the development of operating systems to control the data processing resources of the computer. By the third generation of computers multiprogramming capabilities had made an operating system almost essential. An operating system is a programme that is loaded into the computer every time it boots up which, as well as controlling access to the available resources, supervises the running of other programmes. When first developed, operating systems were linked directly with a certain manufacturers computers but more recently they have been developed by software houses. Standard systems for IBM compatible PCs are MS-DOS and OS/2, both developed by Microsoft, the latter in partnership with IBM. Unix, developed by AT&T in the 1970's, is usable on a number of computer types. Whilst UNIX has the advantage of being a multitasking system a drawback has been the number of different Unix versions available but there are ongoing efforts to produce an agreed standard. Brulé and Chronister estimate that 90% of all chemical engineering software written for PCs is based on DOS, (Brulé and Chronister 1993). The other 10 % are for Apple Mac and Unix systems. Microsoft continue to develop the Windows system, which is DOS based, to include features such as multi-tasking with the latest version being Windows NT. Many users consider that this brings Windows in line with Apple's Mac OS which has been generally acknowledged to be more advanced in terms of ease of use for sometime.

As pointed out by (Ballinger and Anderson 1995) the growth of process

engineering software has in itself lead to the development of languages tailored to suit the needs of the tools, particularly in the area of modelling and simulation. To handle the complexity of the processes being studied these languages are complex and do not as obviously make sense as some of the earlier more general languages. Typical of this type of development is the ASCEND language developed as part of the modelling environment with the same name at Carnegie Mellon University. ASCEND is designed to aid the rapid construction of complex models comprising large sets of simultaneous, nonlinear algebraic equations. The language is object-oriented and consists of two main entities, atoms and models. In more frequently used terminology the models would be considered as classes each containing a number of slots. Each atom has a value associated with it. Features such as inheritance between generations allowing a class hierarchy to build up distinguish ASCEND from languages such as FORTRAN.

2.3.3 User Interfaces

Traditionally the user interface of a programme was taken to encompass only the means of communication with the computer. In the 1950's knobs and dials were used. These gave way to punch cards, followed by keyboard and printer and then mouse and graphics. Keyboard / display and touch screens are currently used for limited applications. The future is likely to be in speech communication and cyberspace tools, such as virtual reality. With each generation of communication more power is required to run the interface. More recently the user interface of a programme is taken to include the input language in which the problem is described, the reporting of results, user documentation and protocols for interfaces with other programmes. To avoid the need for the user to remember commands in whatever operating system language is being used it is usual to have a more user friendly interface. User friendliness is often interpreted as being the ability to input in as natural way as possible with virtually complete transparency of the workings of the software. Results should be usable with the minimum of effort. The graphical environment used depends on the operating system with Windows being used with DOS and Presentation Manager with OS/2. Whilst these are commonly used in PCs, for workstation applications the competing systems are X Window and Display Postscript. X Windows was developed at MIT as a vendor-independent graphical

user interface, GUI, for systems running Unix, (Gunton 1990). Display Postscript and the associated NeWS system were developed by Sun Microsystems for use with the companies workstations.

The advent of PCs running packages such as word processors and spreadsheets under easy to use graphical interfaces has had a great impact on the expectations that people have of computing tools. There is a user led demand for such ease of use from design tools resulting in versions of virtually all commercial tools with GUI's attached. Multitasking and built-in data exchange facilities are two important advantages gained by using Windows.

2.3.4 Databases

A database is a structured store of data containing both the data and the relationships between items of data. The construction and maintenance of databases is carried out by a database management system (DBMS) which is a set of interrelated software tools. Data management within a computer environment for tasks such as payroll control has a long history, but the data involved in process engineering is much more complex than this. Requirements for a DBMS in process engineering are discussed by (Niida et al 1977 and Benayoune and Preece 1987). The latter also give a history of the use of DBMSs in chemical engineering. When looking to the future of process systems engineering in 1983, Motard highlighted the move from programme-centred approaches as a key to making computers useful, (Motard 1983a and Motard 1983b). When discussing the future development of ASPEN Evans points to the integration of database structures as being a key point, (Evans 1980). A properly constructed database system that takes into account the relationship between data items can make the handling of large quantities of data, such as that involved in the chemical plant design process, much easier for the user. Database technology is a key element of integrated engineering systems. This point is highlighted by Kam and co workers whilst describing a process evaluation tool, for the monitoring and analysis of plant performance, (Kam et al 1989). They identify three possible relationships between the data handled, one-to -one, one-to-many and many-to-many. The system implemented is IBM PC/XT compatible based and uses version three of one of the most commonly occurring PC database systems, dBase, with Clipper as the compiler. Winter highlights the emergence of engineering

databases and data exchange standards (see section 2.3.6) as key to establishing integrated computer environments, (Winter 1990). He points to Chiyoda as being pioneers in seeing the potential of databases. To be a success databases need to focus on the more mundane methods of data generation, such as manual calculations, as well as the results of design programmes such as simulators.

Buchmann discusses the problems involved with the development of databases to serve process design (Buchmann 1984). Many of these result from the variety and lack of definition of the data to be handled. The need for revision control and constraint enforcement are also highlighted. Buchmann emphasises the difficulty of someone unfamiliar with the complexity of a field designing an appropriate database structure. This points to the need for an extensively user tested structure unique to each application.

2.3.5 Networks

The reduction in cost of computing power has led to a situation where the vast majority of those working within the process industry have access to PCs on a daily basis. Whilst the number crunching capabilities have freed users from many repetitive tasks there is still a reliance on pieces of paper to transmit data and knowledge between individuals. The much talked of paperless office seems as distant now, for many people, as it ever did. To move away from such a situation requires that data is exchanged in electronic format between computers rather than in paper format between individuals. The first step in achieving this is to move away from stand-alone machines, PCs or Workstations, towards networking. Sawyer describes the background to local area networks (LANs) and highlights three possible network topologies, star, ring and bus, (Sawyer 1990). With the star topology, the simplest, slave nodes communicate with each other via a master which controls access to, and use of, the network. The ring topology has no controlling master and connections are made directly between each node in series. With this system there is an inherent weakness in that the failure of a single node can bring the whole network down. The bus topology also has no master with each node connected over a single open-ended cable. As this topology is easy to extend it has become popular. An example of this topology is Ethernet, originated by Xerox Corporation in 1975, and now commonly occurring in may offices. As a single cable is utilised for multiple nodes it is

necessary to define a protocol for utilisation of the available communication pathways. The most popular protocol, adopted by Ethernet, is carrier sense multiple access with collision detection (CSMA/CD). Here each node listens and transmits only when the network is free of traffic. If a collision is detected, by listening whilst transmitting the node stops transmitting and waits before trying again.

Once data transfer is set-up between the nodes of a LAN it is necessary to consider linking LAN's together. If they are of a similar type a bridge can be used which acts as a mailbox and forwarding address for the nodes in the interconnected LAN's. For dissimilar LAN's a more sophisticated connection is needed which can handle differences in protocol. To avoid communication problems there are three possible approaches; (i) custom-designed interfaces, (ii) adoption of a universal standard or (iii) adoption of a single vendor source. Within the spirit of a free market the last of these is clearly unacceptable. To adopt the first requires a large number of interfaces to be designed. For n different systems n(n-1) interfaces are required meaning 240 to interface 16 systems, (Sawyer 1991). This would clearly place a large development burden on the integration leading to an emphasis on the adoption of a universal standard. This is discussed further in Section 2.3.6.

2.3.6 Data Exchange Standards

The UK PISTEP, Process Industries STEP Consortium, initiative set-up in February 1992 with a budget of £1.8 million and an initial life span of four years was aimed at moving away from the transfer of information on paper towards the use of electronic means. Funding was provided jointly, 50 % / 50 %, by the Department of Trade and Industry and consortium members such as ICI, Shell, John Brown, Foster Wheeler, Intergraph and CADCenter. Membership of the consortium, a total of 17 large companies, represented the full spectrum of process industry companies, operators, contractors and software houses, indicating the generally held importance attached to the field. It should be noted that other industry sectors, notably aerospace and automobiles, are also active in this field and in some instances are considerably further advanced than the process industry. In addition to raising the profile of STEP the main driving force behind PISTEP was the economic benefits that the seamless transfer of technical information can bring, (Sawyer 1993). Sawyer gives a report of the first PISTEP conference held 9th March 1993 and sets out the

aims of the initiative. These were to produce a common industry statement on ISO10303 (STEP) and it's implementation, to position the UK process industry to exploit the competitive advantages of STEP and to establish methodologies for measuring the benefit, (Gardner 1995). In America the equivalent initiative is PDXI (Process Data eXchange Institute), (Sawyer 1992), driven by the AIChemE with industrial sponsorship. A review of PDXI work and methodology is given by (Motard et al 1994). Other countries, and individual commercial organisations, have also been active in this field and to avoid duplication of effort EPISTLE, European Process Industries STEP Technical Liaison Executive, was set up in 1994, (IChemE and IMechE 1994). The initial focus of EPISTLE was the models for activities and data that make up the framework of application protocols for the process industries.

Exchanging data directly between the numerous software tools that can be used would require interfaces between all the systems to be written. To a certain extent this approach is already in place with a number of data exchange standards available. Commonly occurring standards are ASCII, DXF, IGES and SQL. Each have a rather limited range of applicability and are not universally adopted. ASCII is for text. DXF, Data eXchange Format, is the standard used for transferring drawing files between CAD systems. IGES, Initial Graphics Exchange Specification, is an ANSI standard for a neutral file format to transfer data between CAD/CAM systems. SQL, Structured Query Language, is also an ANSI standard but for a high-level language to manipulate data held in relational databases.

Rather than move further down the path of interfaces between individual systems PISTEP adopted the approach of developing a central "hub" containing all the data in a standard formate that can be used by all the applications. Communication is thus between tools and the "hub" rather than directly between tools. This "hub" is the electronic data exchange standard STEP, Standard for The Exchange of Product model data, under development by ISO since 1984. The following advantages have been claimed for the use of STEP, (Sawyer 1993):

(i) Independence from applications and systems with data moved between databases.

(ii) Data can be retrieved and used by people other than the originator who may be working on different systems to the originator.

(iii) All phases of the life cycle of a plant are covered by a single data model allowing integration.

(iv) Data is captured and maintained for at least the life of the plant.

(v) Information products can be managed against an agreed model and standards easing the logistical burden of handling large quantities of data.

As well as data compatibility, to be successfully implemented STEP must address quality assurance concerns and be suited to both the data generation and utilisation methods of the industries being served. Key to these areas is the development of an understanding of how information flows through a project and what form this information will take, leading to the production of a suitable activity model. An early model of this type was developed using the IDEFO modelling method, (Sawyer 1992), but resulted in a static hierarchical view of what is a dynamic process. An alternative, which gives a more graphical representation, is NIAM (Nijsen Information Analysis Method). The development of an activity model for process plant engineering was begun in 1986 by consultant Pat Harrow, (IChemE and IMechE 1994), with subsequent development supported by PISTEP and EPISTLE. The model was designed to give an overview rather than a detailed picture and areas of interest require modelling in a more formal manner before the necessary data management system can be set-up. Underlying the model developed by EPISTLE is an object-oriented framework where generic entity types are used to define the essence of any given object, (IChemE and IMechE 1995b). STEP uses the data definition language EXPRESS and a diagramming convention, EXPRESS-G, to describe the data models, (IChemE and IMechE 1995a). This is a complex task for projects such as process plant design where large and intricate models are needed to represent the data and dependencies involved over the whole lifetime. Setting up such a system from scratch for each project would be prohibitively expensive and thus one of the aims of PISTEP was the generation of an application protocol for process plant. As the PISTEP initiative was drawing to the close of the first phase a second conference was held, March 1995, to review the progress made and look at the way forward. The two major achievements highlighted, (Gardner 1995), were the production of an activity model to give a framework to the application protocol

and the production of a third generation demonstration. The first achievement moves towards the aim of producing a standard application protocol. Whilst the initiative has produced a sound technical basis much work is still necessary to see STEP benefitting actual projects. The feasibility of sharing and exchanging engineering data in the process industries using STEP was established by the demonstrators produced. The first of these came into being in October 1993 after only ten months and established the basic principles. It could be used to create a STEP model from graphical information held in a P&ID file, to view and plot data from a STEP model and query it interactively and to write a STEP file that could be used to exchange data with another system running the demonstrator STEP software, (IChemE and IMechE 1994). This developed into the case study based demonstrator, used at the first PISTEP conference in March 1995, (IChemE and IMechE 1995a). The case study used was a hypothetical North Sea Oil development involving six different partners, each running individual systems, and covering the project life from conceptual design to operation. The development had two main elements, platforms and sub-sea work, each with a different combination of owners and amounted to a capital expenditure of £1.5 billion. At the conceptual design phase the system used was Zyqad's Process Workbench running on PC and Sun Workstation. The information produced was then passed to a Clipper, UNIX based Workstation running PDS for front end design. Detailed design was split into two sections with one part being undertaken using PEGS run on a Silicon Graphics platform and the other performed using a Sun, UNIX, Workstation running RaPID. In line with this split the operations phase was handled using both a Hewlett Packard Workstation running En Garde and a PC running Autoplant. Commissioning and decommissioning aspects were not dealt with. The demonstration illustrated that the increasing quantity of information, in a variety of forms, generated during the progression of a design could be handled without any loss of graphics or attributes. Tracking man-hour savings resulting from the electronic exchange of data gave an overall cost saving of £ 1.3 million for a capital expenditure of £ 1.5 billion. This saving arises mainly from reductions in redrafting and repeated data entry on the project which included 60 PFDs and 2500 datasheets. Initial results from the application of STEP to an actual project with three partners and five systems have been discussed but, due to the early

stage of the project, no serious conclusions could be drawn, (ICheme and IMechE 1996a). Benayoune and McGreavy discuss the integration of STEP compliant tools into a process engineering environment, (Benayoune and McGreavy 1994).

Reflecting on the achievements and looking to the future the PISTEP project manager identified the most important objective as the completion of the data definition as a road to an agreed standard. At the end of the initial four year period, in December 1995, PISTEP continued as a consortium of paying member companies with a focus on short-term collaborative projects addressing business problems where effective data management will provide solutions. No government funding will be used and individual consortium members select those projects with which they wish to become associated. As least one project must be joined and a minimum of 100 hours per annum contributed per project, (IChemE and IMechE 1996a). The level of interest shown given this commitment and the joining fee of £5,000 per annum shows that the importance attached to this field by the process industry continues at a high level. The programme prospectus for this second phase states that the aim is to get over 100 companies of all sizes and from the full range of process industry sectors involved, (PISTEP 1996). Contained within the prospectus are brief descriptions of the twenty two projects initially on offer. These cover data management aspects such as the reduction of the need for redrafting and change management in addition to small practical application type problems such as the purchase of a valve using STEP data and data exchange between in-house systems. All projects demonstrate a strong practical bias in keeping with the PISTEP aim of promoting the application of the technique within the process industry. By mid 1996 30 companies had become members and six projects started, (IChemE and IMechE 1996b). The project areas are: change management, enquiry and purchase, links between process definition and detailed design, maintenance, instrumentation and infrastructure.

2.4 CAD

The acronym CAD commonly has two meanings: Computer Aided Drafting and Computer Aided Design. The latter covers such a wide range of possible applications, from the use of a spreadsheet to size a line to the use of dynamic

simulators to model a complete plant, that it is really of little meaning. Computer Aided Drafting however does cover an easily distinguishable group of tools. Without considering any particular subject area CAD tools have generally been used to replace the drawing board and draughts person / tracer in the preparation of the drawings needed. This covers a whole range of design deliverables such as architectural plans, manufacturing details and cable routing drawings. Within the process engineering field the main application of CAD is in the preparation of PFDs and P&IDs although specification sheet diagrams can also be produced in this way.

Simulation tools such as ASPEN and HYSIM have rather rudimentary graphics capabilities designed to aid the user building models and not to produce graphics of presentation quality. This is illustrated by the decomposition of a PFD to produce a modelling block diagram as shown in the ASPEN plus users guide, (ASPEN 1988). At the next level of detail tools such as Visio and Fast / Easy Process, (Leonardo 1990), are primarily designed to allow individual process engineers to produce drawings, on a PC, that are of suitable quality to be included in presentations and reports. These would, however, be unlikely to be used as the main project drawings for any design due to two main factors. Firstly there is a size limitation of commonly available screens and plotters that makes producing drawings, particularly P&IDs, of suitable quality for general project work by such means difficult. P&IDs contain sufficient levels of detail to require a working size of at least A1. Reduced to A3, the maximum size that can be produced by blowing up the output of a conventional PC printer on a photocopier, normally results in the loss of a sufficient level of detail to make the drawing illegible. The larger size of drawing is necessary to show the plant in sensible sections. Secondly, and possibly more importantly, there is a significant cost impact of using engineers and not draughts people to produce drawings. The former are employed for their design abilities not their draughting abilities and are likely to produce drawings of a significantly lower standard, in a longer time, than the latter. The main CAD packages used in the chemical industry, AutoCAD and Intergraph, are designed for use by dedicated personnel and rows of workstations have replaced lines of drawing boards in most companies. This change has been so generally accepted that it is rare to see hand drawn PFDs and P&IDs today. Perhaps this is a pointer towards the future of hand

done calculations.

Barton and co workers describe a project that they claim as a milestone in the development of CAD use, (Barton et al 1986). A 3-D CAD system, PDMS, was applied during the design of an oil/gas production platform installed in the Gulf of Mexico. Whilst the initial, 2-D, layout was done manually the 3-D model of the plant was used for more detailed layouts, piping GAs and isometrics. The associated database management system allowed the production of reports such as material take-offs. Such intelligent CAD systems are still not in common use with the majority of systems being used purely as drafting tools. Discussing the same CAD system Wheeldon quotes a survey undertaken by management consultants KPMG Peat Marwick that identified project time savings of 20 to 30 % if 3-D workstations are used, (Wheeldon 1992). PDMS was used by BNFL on the Thorp project and Wheeldon reports a claimed overall saving of 25 % arising from increased speed and reduced errors over manual systems. The databases underlying CAD systems, and containing information on components of the design, have the potential to be useful during design to, for example, aid hazard studies and after commissioning to manage modifications and maintenance.

2.5 Process Plant Simulators

The first simulator appeared in 1958 and was developed by the MW Kellogg Corporation. Since then there has been a great expansion in the number and type of simulators available driven by the increases in designers' productivity that comes from increased computerisation of the design process. An early review of process plant simulation was provided by Kehat and Shachan who published a series of articles on the state of this field in 1973, (Kehat and Shachan 1973 a, b and c). They divided simulation programmes into a number of different classes based on applicable processes and mode of calculation. Programmes specific to certain plant types were said to be of equal cost to more general simulators. This is no longer the case and the cost of supporting in-house tools of this type has forced most companies to abandon them in favour of commercial tools. Other notable changes are the incorporation of physical property data packages into all current simulators and the application of increasingly user friendly interfaces. An updated review was given by

Rosen when speaking at a meeting claimed to be the first in America to discuss computer applications in Chemical Engineering, (Rosen 1979). A general review of the background development of simulation is given by (Biegler 1989) who includes a discussion of solution methods. Originally simulators were the preserve of process engineers for use during design. This is now starting to expand to use by control engineers, for operator training and for operator assistance, (Winter 1990). Dynamic simulation is the key to all of these uses with expert systems also needed for the latter.

Before simulation tools containing extensive unit operations libraries and physical properties packages became available the process of computer simulation was much more labour intensive. Crowe and co workers devote an entire book to the setting up and running of a plant simulation using the PACER executive system, (Crowe et al 1971). At this date an extensive staff of programmers and computer operators was required to support the engineer wishing to run a simulation. The executive programme checked that the required information, including calculation sequence, had been supplied by the user, carried out the calculations, via unit operations models, and output the results. Control of the calculation remained essentially in the hands of the user, with the executive acting as a sort of automatic calculator which was particularly useful for processes involving recycle streams. Unless suitable unit operation and physical property methods had been developed previously a significant amount of preparation time was necessary prior to the running of a simulation. Generally the level of process information required limited the use of this technique to modelling existing units.

In an article on work undertaken by CAD Centre, Cambridge, Lessley briefly describes an early commercial simulation tool, CONCEPT, (Leesley 1973). CONCEPT was a suite of programmes with an executive for steady-state simulation. Data was input using a teletyper and consisted of flowsheet structure and connectivity, components present and unit data. CONCEPT contained a library of standard unit subroutines and a physical properties package. Simulation tools can be split into a number of different groups based either on the way in which they perform calculations or the type of calculations they carry out. In the first case there are two main groups, equation based and sequential modular and in the second the split has

traditionally been between steady-state and dynamic simulators. This latter boundary is becoming increasingly blurred with the introduction of tools such as HYSYS where a steady-state model set-up within the environment can be used as a basis for dynamic simulation.

Some senior managers have extremely high expectations of the rise in productivity that will arise from the use of simulators. C. Whitbourne of ICI stated, perhaps with a hint of irony, at a research gathering in 1995 that he wants to move towards a situation where half the engineers can produce twice the work. If such expectations drive the purchase software disappointment is likely to follow.

2.5.1 Solution Methods

Equation based solutions to flowsheeting problems treat the whole plant as a single, large, mathematical problem that can be solved in a single pass using matrix manipulations. The mathematical problem is made up of a set of simultaneous equations that are frequently linearised to aid solution and reduce the computational time required. Numerical algorithms and good initialisation strategies are required for solution. The terms equation based and simultaneous modular are used almost interchangeably by some, but others use the two to distinguish between different solution methods for linearised equation sets. Others identify simultaneous modular approaches as those that resulted from investigations into increasing the efficiency of sequential modular approaches by reducing the degree of iteration. QUASILIN was one of the first tools to apply this method to handle networks of distillation columns. Early academic researchers into process simulation concentrated on this solution method developing, in addition to QUASILIN (Gorezynski et al 1979), approaches that lead to ASCEND and SPEEDUP, (Biegler 1989). Shacham and co workers give a state of the art review of the equation oriented approach to simulation, (Shacham et al 1982). At this date difficulties verifying input data, ordering equations for solution, initializing the vector of unknowns and standardizing the thermodynamic interface prevented the large scale adoption of the approach. ASCEND, FLOWSIM and SPEED-UP were highlighted as programmes based on an equation-oriented approach under development with FLOWPACK moving in this direction. Sequential modular techniques treat each unit operation, or module, as an entity with inputs and outputs and containing the equations necessary to calculate the outputs for a given set

of inputs. Recycle streams must be torn and solved iteratively with the initial estimate provided by the user or as default values. This solution method has traditionally been heavily used in commercially available simulation tools. These tools developed from early simulation work carried out by operating companies, eg COPE at Exxon, FLOWTRAN at Monsanto and SPELS at Shell, (Biegler 1989). The modules making up a process are solved in sequence with the consequent need to provide initial estimates for any recycle streams that are then converged by repeated passes through the loop. Various means of accelerating the convergence of loops are used to limit run times. The difficulty in handling iterative loops is a major drawback of the sequential modular approach. Equation oriented approaches are generally claimed as the means of overcoming the limitations inherent in modular approaches but are not without drawbacks. The main limitation of modular approaches arises from difficulties in dealing with problems where information and material flows diverge. Equation based systems have the advantage that they can be easily extended to perform dynamic simulation and optimisation.

Disadvantages claimed for equation based methods include reliability, difficulty in handling conditional expressions and an inability to monitor the state of individual unit operations during a run, (Best 1989). Evans lists them as the need for a good starting point, the lack of credit for sequential modular models developed for unit operations by industry and difficulties in detecting errors, (Evans 1980). He claims rapid convergence as a positive point. Best goes on to claim that a modular technique, especially a parallel one, may be most useful for dynamic simulation. Two-tier solution methods using simple and rigorous models are claimed to overcome the disadvantages of equation based solutions, (Evans 1980). Simple models are in the form of approximate equations that can be easily solved to provide the stream variable values to be used in the rigorous models. These latter models are typically unit operation models as used in sequential modular solution methods. Simultaneous modular approaches where unit operation modules remain intact but stream connections are solved simultaneously blur the distinctions between the two simulation methods.

2.5.2 Simulation Types.

Due to the complexity of modelling dynamic behaviour the first simulators

to be developed and used extensively were steady-state. However these simulators provide only a partial picture of plant behaviour and give no insight into aspects such as start-up and disturbance rejection that are crucial to satisfactory plant performance. When looking at control system design for distillation processes, Karlstrom and co workers conclude that it is necessary to consider dynamic behaviour from the earliest stages of design if a satisfactory solution is to be reached, (Karlstrom et al 1992). This conclusion is borne out by industrial case study material reported by (Bouwens and Kostes 1992). They discovered that the system configuration ranked last when control system design followed equipment design, but was the most favoured option when design was integrated. Dynamic simulators have been developed to deal with such situations but are still not yet commonly used despite a long period of academic interest. Moe and Hertzberg claim that lack of computing power has been a significant hold on the wide scale adoption of dynamic simulation (Moe and Hertzberg 1994). They review work on advance computer architectures aimed at overcoming this and point out that simulators designed to run on conventional computers are not easily adapted. The speed of adoption of advanced computer environments will in itself act as a barrier. Dynamic control studies were first carried out in the 1950's on analog computers and by 1980 a second generation dynamic simulator, DYNSYL, aimed at the nuclear industry had been developed, (Patterson and Rozsa 1980). DYNSYL was reported to have interactive elements in requesting information such as time intervals and changes to be made from the user but the mode of inputting, limited range of models and lack of significant graphics capability would not satisfy current standards of user friendliness. Part of the reason for the slow up-take has been the quantity of data needed to run dynamic simulators. Dynamic simulation can help to improve understanding of the mechanisms involved in a process and, for existing processes, help identify debottlenecking potential. To get the greatest benefit from dynamic simulation it should be undertaken as soon as adequate design information is available so that the results can be incorporated into the design. A review of the early development of these tools is given by (Biegler 1989) and a state of the art review by (Pantelides and Barton 1993). Depew and Nielsen claim that the evolution of equipment configurations and control schemes that result from the use of dynamic simulation leads to benefits during plant start-up,

(Depew and Nielsen 1996). These benefits arise from a reduction in field changes for a design validated in this way, testing of start-up and shut-down sequences and the provision of controller tuning parameters. An early practical application of dynamic simulation is described by Hudson who deals with the modelling and analysis of a North Sea oil and gas production facility, (Hudson 1991). The model was built by a sub-contractor and passed to the design contractor who found it useful for testing operating procedures and alternative control system designs. On the completion of the design phase the model continued to be available as an aid to the commissioning team. This multiple phase usability of dynamic simulation is also emphasised by Fidgett and Harrison who describe early work at BNFL in the development of such simulation of an effluent treatment plant, (Fidgett and Harrison 1989). Naess and co workers give a review of dynamic simulation usage within Norsk Hydro, (Naess et al 1993). They emphasise the benefits in information flow that have arisen from the dynamic tools from feasibility through to plant operation and claim that it has helped to reduce project costs and timescale. Examples of real applications at various project phases are included.

One area where the use of dynamic simulation is relatively well established is in the field of operator training, although the early optimism as expressed by (Dixon 1991) has been some what diluted as the costs of ambitious training programmes have become apparent forcing scaling down. The use of simulators for training was pioneered in the aviation industry where the dangers of letting untrained pilots practise on real, highly expensive, planes are obvious. As process plants are also expensive and potentially dangerous advantages in terms of reduced down time and more efficient operation should be gained by the use of simulator based training. Unfortunately such advantages are difficult to quantify, complicating the economic case for investing in the development of a training simulator. Bretelle and co workers propose a training system that links the dynamic simulator SPEED-UP with an industrial control system to give a real time response, (Bretelle et al 1994). A prototype based on a batch PVC polymerisation process is described which also includes a scheduling tool, SUPERBATCH. No industrial applications are mentioned.

2.5.3 Range of Applicability.

The big commercial simulators such as PRO II, ASPEN plus and HYSIM claim to be applicable to a wide range of plant types. There are however a far larger bulk of tools that have been developed specifically for a given type of simulation. Lattas and Marktos mention such a tool, AGaPSS, for the simulation of gas sweetening plants using amine solutions, (Lattas and Marktos 1989).

2.5.4 Available Simulators.

There are a large number of simulators available, some for general use and some for specific applications. The number of tools available, each with different strengths and weaknesses, can make comparison and selection difficult for users. Rippin reports on efforts by the EFCE Working Party on the Use of Computers in Chemical Engineering to establish standard test problems for simulators, (Rippin 1983). These problems were designed for relative ease of setting up but to be sufficiently demanding to act as tests of aspects of tool performance such as unit operation models and ease of inputting a new model description. Results of the comparison test are not included. Leesley and Pollicoff also designed a problem to be used to test simulators, as an aid to the selection of an appropriate tool, (Leesley and Pollicoff 1982). They specifically focused on areas known to cause problems for simulators.

Commercially available simulators and the extent of their use is discussed in Chapter 3 but practical descriptions of various tools are included here.

2.5.4.1 ARACHNE.

ARACHNE, A Reactor And Cycle Handling Network Evaluator, was development by British Coal's Coal Research Establishment, CRE, during the 1980's for the evaluation of coal utilisation technologies, (Topper et al 1989). Whilst the architecture and solution methods employed by ARACHNE were not unusual the area of applicability required that it should be capable of handling solids and three phase systems. These systems have generally been poorly covered by the most commonly used simulators. In addition to a suitable library of standard modules set up to model the required phases, ARACHNE used the concept of pseudo-components to characterise chemically ill-defined materials such as coal.

2.5.4.2 ASCEND.

ASCEND is an equation oriented simulator developed by Westerberg and co

workers. Locke and Westerberg describe the capabilities of ASCEND-II, (Locke and Westerberg 1983), which is described as an interactive equation based flowsheeting system capable of undertaking performance, design and optimization calculations. Interactive programmes are claimed to reduce the chances of users making potentially expensive errors in input values. Cost and time savings are also claimed to result from the integration of simulation and optimisation. Equation based systems can be more easily extended to perform dynamic and optimisation calculations than sequential modular tools and this feature was utilised in ASCEND-II. The interactive capabilities of ASCEND-II allow the user to evolve a problem solution by adding complexity, e.g. in physical property methods and unit operation models, as and when appropriate. Initial runs would be simple, steady-state simulations without optimisation which, if they ran successfully, would then be re-run with increasingly complex models and calculation types. The capabilities and structure of ASCEND-II are described in detail by Locke and Westerberg. Piela and co workers discuss the ASCEND modelling language developed for the implementation of ASCEND, (Piela et al 1991).

2.5.4.3 ASPEN plus.

ASPEN (Advanced System for Process ENgineering) was developed at the Massachusetts Institute of Technology during the late 1970's, (Evans et al 1979). It was developed as a sequential-modular simulator due to familiarity with this type of solver but was designed to permit extension to a simultaneous modular architecture when this had been proven. Work was supported by the U.S. Department of Energy to allow the development of a tool for use in the engineering fossil energy conversion processes. It was one of the first simulators with a solids handling capability. The use of ASPEN plus for solids handling processes is described by (Evans 1989). Extensive industrial collaboration was also key in the development and guided key choices such as architecture and language. Experience gained during the development of ASPEN are reflected in the review paper due to Evans, (Evans 1980). Due to the emphasise on energy conversion processes rather than petrochemical processes during the development of ASPEN considerable emphasis was placed on the representation of streams. These can be conventional, for components characterised by commonly occurring physical properties, non-

conventional, for items such as coal, or information,used for heat flows, (Evans et al 1979). This work is reviewed by (Britt 1980). ASPEN determines the computational sequence to be used during the solution and uses an accelerated form of the Wegstein method to converge recycle streams. FORTRAN was selected as the language to implement ASPEN due to the portability afforded and the high level of experience available in most companies. Initially ASPEN utilised many FLOWTRAN unit operation models. Subsequently a second generation tool, ASPEN plus, has been released using models developed specifically for the tool. The flexibility of ASPEN plus has resulted in its' use as the basis for a number of more specific tools. Farag and co-workers describe the development of models within ASPEN plus to allow the simulation of waste water treatment processes, (Farag et al 1990). Other modelling applications are as diverse as life support systems for space craft (Modell et al 1989), the retorting block of an oil shale conversion process (Dung and Benito 1990), polymer manufacture (Ko et al 1992), Ethanol production processes based on enzymatic hydrolysis of woody biomass (Galbe and Zacchi 1994), electrolytic process optimization (LaRoche et al 1994) and the production of Methanol from natural gas (Dave and Foulds 1995). Eriksson and co workers report on trials to use ASPEN for the simulation of kraft pulp processes, an area where MASSBAL and GEMS are more frequently used, (Eriksson 1994). Simulation results were tested against data collected from an operating plant. Problems were encountered as the ASPEN data bank did not include some of the components necessary and also in achieving sufficiently accurate models of some of the none standard unit operations. Additional FORTRAN coding would be necessary to achieve this. This range of reported applications shows that ASPEN has gone a long way towards the original development goal of extending process simulation to cover a broad range of processes.

2.5.4.4 GMB

GMB (General Material Balance) was developed by the contractor Badger as a simulator starting in the early 1960's, (Russell 1980). It was a steady-state sequential modular simulator, written in FORTRAN, with calculation steps called actions and not blocks. Rather than adopting the preprocessor type architecture common to most simulators, all parts of the programme were pre-linked making the

addition of models difficult. Russell claims the advantage of this architecture as being a reduction in the overhead associated with compilation of each run. Given advances in computing capabilities it is doubtful if this would now out weight the inflexibility of being unable to extend. GMB used a single data management subroutine to control data handling, storing all problem data and moving it into the working area as necessary. Inputting was via, what now appears to be very dated, coding sheets where blanks were filled in. This was claimed to reduce the chances of errors and omissions. The user was responsible for specifying the calculation sequence and recycle streams but the programme did check for errors. Some level of interactive capability was included by the option to interrupt runs and alter parameters. Whilst now looking old fashioned GBM contained many elements that now commonly occur in simulators, the architecture however has not endured.

2.5.4.5 FLOWPACK

After development and use by ICI, in the early 1970's, the German contracting organisation Linde acted as a partner with ICI in the development of FLOWPACK II. The development is no longer supported by ICI who now use commercial simulators ASPEN and PRO/II. Berger and Perris discuss the development of the FLOWPACK II system, (Berger and Perris 1979). FLOWPACK II is a steady-state simulation package designed to be applicable to a wide range of process types, including solids handling, and over a range of project types, from conceptual mass balances to debottlenecking of existing plants. The basic criterion to be satisfied during development is stated by Berger and Perris as:

"The minimum total expenditure of manpower and computing resources to derive a satisfactory solution to the problem, within the timescale dictated by the project."

This overall criterion masks sub-objectives that define items such as the requirement for computational efficiency, ease of use, range of use and extensibility. Ease of use is highlighted as an area that required a considerable amount of effort to ensure that the system freed the user from tedious aspects of their job without being irksome to use and encouraging creativity. Interactive data preparation and limited interactive capabilities during a run are highlighted as desirable attributes. The preparation of a dynamic simulator based on FLOWPACK II has been reported.

2.5.4.6 FLOWTRAN

FLOWTRAN is a sequential modular simulator that requires the user to supply the computational sequence. FLOWTRAN (FLOWsheet TRANslator) was developed by Monsanto during the mid 1960's, going on internal general release in April 1966. External licensing followed in the early 1970's. The FLOWTRAN system consists of an integrated set of programmes, written in FORTRAN to aid portability, (Rosen and Pauls 1977 and Larsen 1982). The components of the system are as follows:

(i) FLOWTRAN Process Simulator. This translates the description of a flowsheet into a programme which is then executed.

(ii) PROPTY Physical Property Program. This takes raw property data and computes the constants for the correlations used by the simulator.

(iii) VLE Phase Equilibria Program. Similar to PROPTY but computing parameters for the liquid phase activity coefficient correlations from raw phase equilibrium data.

(iv) INF Information Retrieval Program. This stores the constants produced by PROPTY in a data file and retrieves them for use by FLOWTRAN.

In the late 1970's the following information was needed by FLOWTRAN in order to undertake steady-state simulation of a plant, (Rosen and Pauls 1977):

(i) The name and type of each unit operation.

(ii) The order of calculation.

(iii) The name of the input and output streams from each unit.

(iv) The chemical components present.

(v) Key unit design and operating variables, eg heat exchanger areas.

(vi) The composition and conditions for each stream flowing into the plant.

As well as the operating conditions for each unit and stream compositions and conditions economic data such as unit costs could be obtained. The data required is very much the same for simulators today, with the exception of the need to supply the calculation sequence, but the style of input, free format onto a blank screen, would no longer be considered user friendly. In general FLOWTRAN unit operation

blocks calculate outputs for a set of inputs but the incorporation of control units allows the monitoring of a variable and the manipulation of upstream parameters to achieve a particular value. As the order of calculation is user specified recycle streams must also be torn by the user. A convergence unit must be specified to allow solution of the recycle from the initial estimate. Neville and Seider extended the capabilities of FLOWTRAN to solids handling equipment in the coal gasification process by incorporating FORTRAN routines from PLEXSYS, (Neville and Seider 1980). In 1977 FLOWTRAN was licensed to MIT for use as a basis for developing ASPEN, (Larsen 1982).

Abatzoglou and co workers report on an application of FLOWTRAN in the pulp and paper industry involving solids and inorganic compounds, (Abatzoglou et al 1990).

2.5.4.7 MASSBAL

MASSBAL was developed to address the simulation needs of the pulp and paper industry where difficulties in defining physical properties and unit operations were found to lead to poor performance of more general simulators, (Shewchuk 1982). Initially a limited number of unit operations were included and had to be combined to model process equipment. Also no physical property library was included with the user having to supply such data. Data input was via the use of keywords. Subsequent revisions have refined the facilities available and have moved towards more general applicability. MASSBAL 3.0, announced in 1993 (Kernan 1993), includes dynamic simulation capabilities and physical property methods.

2.5.4.8 MASTEP

MASTEP is a modularely organised steady-state simulator developed in Hungary for use in process research and development, (Timár et al 1984). Sequential and simultaneous equation solving modes are combined with a number of convergence methods within MASTEP to give the user computational flexibility. Preliminary calculations, involving mass balance only, or rigorous analysis, with heat and mass balances, can be performed. Timár and co workers claim four to six industrial simulation tasks per month carried out using MASTEP. The executive programme for MASTEP was written in FORTRAN but, showing the age of the tool, the user interface was written in BASIC.

2.5.4.9 PACER

PACER was a modelling system used in the early 1970s as a forerunner to simulation tools. Compared to current simulation tools the facilities were very primitive with the user expected to undertake a high level of model development and to input to the solution strategy, (Barker and Leather 1972). The unstructured nature of the data generated was viewed as a problem even then and a report writer per unit was suggested as a means of overcoming this.

2.5.4.10 PRO/II

PRO/II is a sequential modular simulator that SimSci introduced in 1990 to supersede PROCESS. It is a general purpose steady-state simulator which can be used with the PROvision GUI to ease the building and modification of models. The target industries are refining, gas processing, petrochemicals, chemicals and contracting. To service this, PRO/II contains a wide range of unit operations models including a number of options for distillation, heat transfer, reaction and solids handling. To support the unit operation models PRO/II has extensive physical property capabilities. Capabilities highlighted in promotional literature for PRO/II are the ability to handle electrolyte chemistry, non-ideal distillation, a wide range of reactive systems and vapour/liquid/solid separation systems.

2.5.4.11 PROCESS

PROCESS was a sequential modular simulator developed by Simulation Sciences Inc. during the late 1970's, (Brannock et al 1979). It has subsequently been superseded by PRO/II. The programme was written in FORTRAN and was a steady-state tool aimed at the chemical, petrochemical and synfuel industries. Runs were executed in batch mode with inputting, preprocessing and output examination carried out separately to the simulation. Recycle tear streams and calculation sequence were determined by the programme. Latterly PROCESS could be customised to allow integration with a drafting tool.

2.5.4.12 SpeedUp.

SpeedUp is a commercial dynamic simulator based on work undertaken by Sargent and co workers at Imperial College and is currently marketed by ASPEN. It commenced life in 1958 as a steady-state simulator and did not include dynamic capabilities until the 1980s, (Sargent et al 1982). SpeedUp is, unlike the majority

of commercially available simulators, an equation based simulator with both steady-state and dynamic simulation capabilities. It can also undertake optimisation. Conceptually it consists of two parts: a translator / command executive and a FORTRAN run-time system. The equations to describe the problem are assembled by SpeedUp using information on flowsheet topology and unit operation models. The user defines a SpeedUp problem using free-format interactive input and keywords, (Sawyer 1991). If no input errors are found a FORTRAN programme is then constructed and solved by the run time system. The time taken for the translation is largely dependent on the complexity of the flowsheet. Steady-state simulation is treated as a special case of dynamic simulation with the time derivatives in the models used set to zero. Barton and Perkins claim that SpeedUp offers advantages in the field of minerals processing due to flexibility in problem specification and the ability to handle plant dynamics, (Barton and Perkins 1988). A limitation is the inability to handle partial differential equations leading to the need for alternative model formulation in some cases. Updates of the original programme are described by (Pantelides 1988). These include the ability to use numerical and symbolic information in the solution algorithm. The ability to investigate process and control scheme interactions is one of the benefits of SpeedUp but the computing power required for utilisation is significant.

2.5.4.13 QUASILIN

QUASILIN is an equation-oriented simulator originally steady-state but subsequently modified to become dynamic, (Smith and Morton 1988). The work was undertaken at the University of Cambridge. Within QUASILIN a process is set-up as a set of non-linear equations representing the units and stream connectivity. For dynamic simulation differential equations are included. At the time of writing dynamic models of mixers, flashes, reactors, pumps, valves, compressors, pipes and controllers were included within QUASILIN. Other unit operation models were pulled from the steady-state simulator base. The equations are solved by an iterative linearisation process, usually involving the Newton-Raphson method. To run a dynamic simulation problem the user supplied input file is translated to a FORTRAN programme and a data file by the input processor. These are passed to the main executive that calls the relevant units to set their equations as appropriate. The

equation set is then solved. Interrogation of the considerable quantity of data produced then takes place off-line. Graphical and tabular analysis is integral with QUASILIN to help the user handle the quantity of data involved.

2.5.5 Future Developments of Simulation.

The increased use of graphical interfaces has made simulators much more user friendly and has helped ensure their general acceptance. Performance must now be improved.

The development of tools capable of handling batch plants and dynamic simulation means that much more realistic modelling of an operating plant can now be achieved than ever before. Still a gap remains between simulation and plant operation. Currently simulators are mainly design tools used by process engineers not directly involved in the day-to-day running of plants. Increased processing speeds combined with the development of dynamic simulators have allowed close to real-time responses and the development of simulator based operator training. Bailey and Matzopoulos point out that as dynamic models are expensive to build and maintain, simulators that move from the design phases to the operating phases are required, (Bailey and Matzopoulos 1996). In addition to operator training such tools should be capable of supporting the development of the operating plant by capturing knowledge, improving understanding and allowing evaluation of improvement ideas. They term such tools multi-purpose operations simulators and describe such a system developed for a BP Exploration oil field site in Colombia. Rather than emulate the plant control system in the simulator the system architecture used directly connects a copy of the plant control system to a simulation of the process only. This arrangement allows changes to the control algorithm to be incorporated into the simulation without the need to modify the plant model.

One possible advance is to develop the use of real-time simulators using plant data to provide on-line optimization, representing an additional step towards automatic plant control. On-line optimization will enable a plant to operate at close to optimal performance and hence provide a competitive advantage. A collaboration between Shell Oil and Simulation Sciences to produce such a system, ROMEO, is currently under way, (Anonymous 1996). Much of the technology necessary to support such systems is already in existence. Systems for the real-time collection of

plant operating data have been commonly in use since the 1980's, although they were available in the 1970's, and form one of the basic blocks for a real-time simulation system.

2.6 Expert Systems.

During life a human being accumulates knowledge from a large number of sources and in a wide variety of formats and then uses this knowledge to deal with situations that are later encountered. Intelligence can be defined as the ability to bring knowledge to bear on actions to attain goals, (Newell 1980). If no direct comparison can be found then extrapolation is used in order to determine an appropriate response. The level of knowledge about any given subject rises with exposure to that subject and after a certain point is reached a person may then be termed an expert to whom others refer for guidance. Expert systems are attempts to capture the knowledge held by human experts and formalise it in a computer tool that is available for consultation at all times. The capture of the knowledge is one of the most difficult aspects of the setting up of expert systems, although it has been suggested, (Rogers and Petry 1995), that, using an expert system shell, an engineer familiar with computers could build such a system using knowledge acquired from books etc. The desirability of such a situation is questionable given the conflicts that could arise and the potentially incomplete decision basis.

Expert systems commonly contain two basic elements, the knowledge base containing information specific to the problem domain and the inference engine that guides the use of the knowledge, acquires information from the user and controls the reasoning process. These can be essentially independent or coupled. Additionally a user interface, explanation facility and knowledge acquisition module are necessary. In conventional computer programmes the data base and code are integrated but in expert systems the knowledge base and means of controlling the search are separated. Changes in knowledge then require only changes in the knowledge base. Knowledge encapsulation works well for some knowledge types but there can be significant problems leading to a limited applicability of expert systems. Background information on expert systems is included in (Rogers and Petry 1995). Whilst discussing the automation of HAZOP Kletz identifies four types of knowledge that

would have to be captured by an expert system, (Kletz 1992). Plant specific knowledge could well be captured but the effort would not be worth the while for the limited number of studies to which it would be applicable. General process engineering knowledge constitutes a large bulk of information that could be captured if sufficient time were available. General scientific knowledge falls into the same category but the task would be prohibitively large for a truly general system. Everyday or common sense knowledge is the least structured of the four types and would not be capable of capture by available techniques. Beltramini and Motard also split the knowledge used by process designers into four classes but along the lines of data source, (Beltramini and Motard 1988). The classes are: Data obtained from laboratory experiments, general data from standards and specifications, data produced by mathematical models and heuristics and judgemental knowledge. This latter category is the domain of expert systems. Beltramini and Motard proposed a knowledge representation system, KNOD, to handle this type of knowledge. Expert systems commonly use production, if-then, rule or object oriented knowledge bases.

Expert systems are commonly referred to as either shallow or deep. These terms relate to the knowledge used in setting them up. Shallow expert systems use rule based knowledge such as that developed by operating experience of a plant. They have limited ability to explain why a particular solution was selected and can only solve problems of a type encountered previously and encoded. Deep expert systems contain more fundamental knowledge about a system that can be used to reach a decision about novel problems encountered. There are a number of ways of capturing deep knowledge including using models of the system and fault trees. Key to expert systems is the use of exploratory problem solving techniques. In complex problems the number of possible solution paths can be very large, therefore to be effective heuristics are used to constrain the search. The inference engine provides the logic for reaching conclusions within the expert system. There are two main forms of logic inference used, backward and forward chaining. Backward chaining starts with the conclusion and sets out to determine if it follows from a given set of facts and rules. Forward chaining starts with a known fact or rule and attempts to reach a conclusion. The latter is closer to the way in which a human would tackle the problem. Various methods aimed at increasing the efficiency of problem solving

by inference are described by (Rogers and Petry 1995).

A precursor of expert systems within the process industry was the use of structured checklists such as the application discussed by (Wells et al 1989). Here a structured checklist, executed using Lotus AGENDA, is used to aid the identification of the root causes of faults and errors on chemical plant. The process industry has, however, been far from the forefront in realising the potential of expert systems. Andow identifies the terminology employed in the field and the lack of demonstrable practical applications as being key in the slow uptake. Early leaders in the field were medicine, with diagnostic tools, and the Nuclear Industry. Civil engineering has also participated. Early work specifically related to the sub problem of structural design is reviewed by Sriram and co workers, (Sriram et al 1985). A more sweeping approach is adopted by Bédard and Gowri who address the problem of automating the complete problem of building design using KBES, (Bédard and Gowri 1990). They include a count of KBES tools in operation at the time and point out that the majority are for diagnosis, monitoring and interpretation rather than for design. Whilst Bédard and Gowri claim that building design is unique the characteristics listed as a basis for this uniqueness are very similar to the characteristics of chemical plant design; a single product in a natural environment, contributions from several disciplines and composition of subsystems that need to interact. They identify the integration of different parts as being a key to designing better buildings along with the availability of expertise during the preliminary stages of the design. The same is true for chemical plant design therefore if a KBES can be developed for building design one should also be possible for chemical plant design. Due to the range of problem types in plant design the problem is however more complex.

The development of expert systems for chemical engineering is discussed by (Bunn and Lees 1988) and (Niida et al 1986). A comprehensive review is given by (Stephanopoulos and Han 1996). Bunn and Lees focus on the design of plants handling hazardous materials at the conceptual phase of design. Their aim being to examine how expert systems can aid the incorporation of inherent safety into design. Areas focused on were emergency isolation, flare systems, pressure relief systems, valve sequencing, fault propagation, fault tree synthesis, hazard identification and

alarm diagnosis. Issues relating to the implementation of expert systems for all these areas are discussed including sources of relevant knowledge for capture. Niida and co workers point to CONPHYDE and HEATEX, developed at Carnegie Mellon as being early players in the field of expert systems applicable to process engineering, (Niida et al 1986). At that time no reports of process engineering expert systems in practise had been published. Niida and co workers developed four experimental expert systems in the fields of: synthesis of P&IDs, selection of inert gas generation processes, determination of distillation sequences and determination of distillation control systems. A number of knowledge acquisition techniques were employed including question and answer sessions, the use of company technical documentation and papers / reports unearthed by literature survey. The knowledge acquired was expressed as tables or heuristic rules, written in natural language, during encoding. Tomita and co workers report on work to encapsulate operators knowledge into a system to synthesise plant operating procedures, (Tomita et al 1989). In another field of process engineering Crowe and co workers describe the development of an expert system for whole plant process synthesis, (Crowe et al 1992). They point out that procedural languages, such as FORTRAN, are not of much use in developing expert systems due to the inability to support dynamic data structures or symbolic manipulation. Reflecting on the suitability of expert systems for discrete tasks Santon and co workers report on work supported by the HSE to develop expert systems for the sizing of relief vents for dust explosions, (Santon et al 1991).

One area where there has been a considerable amount of work reported on expert systems is in process plant fault diagnosis. A review of the issues involved and some of the early work is given by (Moore 1986). The issues identified by Moore are:

(i) How to handle the large number of measurements involved, given the possibility of rapid change and the need to service trending.

(ii) How to represent the large knowledge base necessary for a plant.

(iii) The need to provide real time advice or control actions, particularly during an emergency situation.

(iv) How to provide AI expert backup to service the system.

(v) How to test that the knowledge base is consistent and complete.

Moore proposes PICON (Process Intelligent CONtrol) to address these issues. This can handle up to 20,000 measurements with a real time interface for the operators

Adamson and Roberge describe the preparation of an expert system for use in fault diagnosis in the nuclear industry, (Adamson and Roberge 1991). They point out that increasing complexity and automation have made such diagnostic systems increasingly important in many fields. This view is shared by Winter who identifies the provision of operator assistance using a combination of simulation and expert systems as a future area of expansion, (Winter 1990). On the same theme Rich and Venkatasubramanian describe a prototype expert system, MODEX, for locating the causes of faults on process plant, (Rich and Venkatasubramanian 1987). MODEX (Model Oriented Diagnostic EXpert) was based on a variant of the fault tree synthesis technique and employed deep knowledge to be generally applicable. The model-based system used was subsequently found to lack diagnostic efficiency and an improved system, MODEX2, has been proposed, (Venkatasubramanian and Rich 1988). MODEX2 integrates compiled knowledge, based on past experience, with deep-level knowledge, based on fundamental principles and applicable to all situations. A two tier knowledge base architecture is used with complied knowledge as the top tier and deep-knowledge underneath. Shum and co workers adopt a different approach to malfunction diagnosis on chemical plants, (Shum et al 1988). They utilise knowledge embedded in a hierarchy of nodes which is claimed to mirror the way that a human expert would tackle problem solving. Nodes higher in the hierarchy are associated with general malfunction hypotheses and those beneath, representing a greater level of detail, only being investigated if those above have been established as valid. This reduces the search area. Each node contains the knowledge necessary to establish or reject it as relevant to the malfunction under investigation. This effectively integrates the knowledge base and inference engine which complicates the updating of knowledge by forcing each node to be addressed separately. Sum and co workers claim that complete separation of the two elements is unlikely to be a viable basic principle for the organisation of expert systems. The prototype system described is specific to a small part of a plant and it is not clear how much effort would be necessary to construct a diagnostic system for a complete

plant though it appears that each application would require separate treatment. Lapointe and co workers describe BIOEXPERT, a prototype expert system with a focus on fault detection and diagnosis for waste water treatment plants, (Lapointe et al 1989). The intent behind BIOEXPERT is to provide an on-line tool to aid the operator by encapsulating the knowledge used by the process engineer during diagnosis. Due to problems in obtaining on-line readings for some properties of biological streams completely automated data inputting would not be possible. At the time of writing BIOEXPERT had only been applied to pilot plants with most data manually input via a menu system. In addition to the input menus BIOEXPERT contains an expert system shell, written in Prolog, a database and an explanation facility. This latter section is emphasised as important and explains both how conclusions were reached and why data has been requested. BIOEXPERT performs diagnosis using the hypothesis-test strategy adopted by humans when tackling such problems. Shallow knowledge is used to direct the search. Saelid and co workers report on an industrial application of an expert system diagnostic tool, (Saelid et al 1992). Poor environmental discharge performance at a Norsk Hydro fertilizer plant in Norway prompted the development of a tool that was aimed at supporting the operator by detecting, diagnosing and reporting non-optimal plant behaviour. A GUI was used to flag deviation messages and to track the progress of the diagnosis.

Bañares-Alcántara and co workers review the applicability of knowledge-based expert systems (KBES) to the field of chemical engineering, (Bañares-Alcántara et al 1985). They identify seven classes of problem type encountered by chemical engineers where KBES could be applied. These cover the spectrum from derivation, identification of a path to a known solution, to formation, search for a solution within problem constraints. Systems in fields related to process engineering mentioned by Bañares-Alcántara and co workers are as follows:

(i) HEURISTIC DENDAL. To help chemists determine the molecular structure of organic compounds. This is highlighted as laying the foundation for the development of many rule-based expert systems.

(ii) FALOCN. For diagnosing faults in process plant.

(iii) CONPHYDE. A system for identifying the most suitable vapour-liquid equilibrium method for mixtures of compounds. The development of this tool

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is described by (Bañares-Alcántara and Westerberg 1985), the aim being to evaluate the feasibility of applying AI techniques in the Chemical Engineering area. A successful prototype of this well defined area was developed based on an existing expert system from the geology field, PROSPECTOR. Paranjape and Kudchadker also propose a tool, CHOCOVALE (CHoice of COrrelation for VApour-Liquid Equilibrium computations), in the same area, (Paranjape and Kudchadker 1993). A more advanced expert system for physical property selection is reported by (Gani and O'Connell 1989). Here optimal models for a number of properties are selected for specified mixtures.

(iv) PICON. For monitoring and controlling industrial processes.

(v) HEATEX. For aiding in the construction of heat exchanger networks.

(vi) DECADE (Design Expert for CAtalyst DEvelopment). To aid a user in the selection of a catalyst for a specified single-step reaction. The basic development of this tool is described by (Bañares-Alcántara et al 1987). At this stage the specific area of knowledge encapsulated in DECADE was hydrogenation of carbon monoxide.

Looking to the future Bañares-Alcántara and co workers saw an expansion in the use of KBES in process design which has not yet appeared in commercial tools although research in this area continues to be active. Other reported applications of expert systems are mentioned below. Lahdenperä and co workers discuss a prototype expert system to aid in the selection of solid-liquid separation equipment, (Lahdenperä et al 1989). Kirkwood and co workers report on the development of PIP (Process Invention Procedure), an expert system for the synthesis of chemical process flowsheets, (Kirkwood et al 1988). An hierarchical methodology using qualitative and quantitative knowledge is employed. In the same field Wahl describes PRINCE, a system to aid in the selection of refinery process units to meet feedstock and product specifications, (Wahl 1994). As well as an expert knowledge model graphical data is used as appropriate. In the field of equipment selection, specifically aimed at the conceptual phase of design, Yang and co workers describe heat exchange equipment (HESES) and liquid mixing equipment (MIXES) tools, (Yang et al 1993). Beiker and Simmrock mention a raft of tools in this field, PROSYN,

and describe SOLPERT, for the selection of mass separating agents for extractive and azeotropic distillation in detail, (Beiker and Simmrock 1994). SOLPERT implements a four step hierarchy of increasing detail. First the class of solvent is selected, followed by the selection of the chemical group, the functional group and finally the proposed solvent. Other expert systems within the distributed PROSYN system cover rectification and heat integration. Schembecker and Simmrock describe another tool, AZEOPERT, implemented within PROSYN, (Schembecker and Simmrock 1995). AZEOPERT uses data base searches, heuristic rules and numerical routines to predict azeotropic behaviour. A more general view of PROSYN is given by (Schembecker et al 1994b). Yorke and co workers describe the development of an expert system for the on-line monitoring and control of beer fermentations, (Yorke et al 1996). This demonstrates a process industry use of expert systems that moves beyond design assistance and into operating assistance. Basila and co workers report on the use of an expert system for the real time control and fault diagnosis of a chemical plant, (Basila et al 1990). The prototype system proposed, MOBECS, adopts an object based knowledge representation. This is claimed to be the best representation for real time systems. An example of the use of the system to monitor and control a packed-bed reactor system is given but it is not clear how much work would be involved in setting up the knowledge base for each new application. A review of expert systems in the safety design field is given by (Rogers and Petry 1995).

Expert systems can never completely replace an expert but, by allowing more mundane and routine applications to be carried out by less experienced staff, free the expert to deal with the more complex cases, (Androw 1988). Androw looked to the future of the application of expert systems to process design and saw a move away from systems designed for specific tasks, such as valve selection, towards more general applications such as fault diagnosis and operations planning. Other areas of possible change were identified as improved interfaces and levels of explanation, increased integration of systems and an increased number of intelligent products. Advantages foreseen were a reduction in errors, increased creativity, increased productivity, safer plants and more on-specification products, (Androw 1988). These are sweeping claims and after eight years there is little evidence to justify such optimism. Becraft and Lee describe a fault diagnosis system that combines expert

system and neural network elements to overcome the disadvantages inherent in each, (Becraft an lee 1993). The expert system strength of good explanatory facilities are utilised along with the increased ability to handle novel situations exhibited by a hierarchical neural network structure.

2.7 The Future.

One frequently discussed element of computer technology that is supposed to be poised to revolutionise the way that people work is the Internet or "information super-highway". Whilst this is currently undergoing rapidly expanding usage security concerns have so far acted as a break on serious commercial exploitation of the medium. For the year 1992 the traffic amounted to 500 million bytes rising to 13,000 million bytes in 6 hours on 10th November 1994. Visions of the future include control of plants via the Internet, (Lane 1996), with PCs and workstations replaced by simple, small, portable I/O devices capable of communicating with much more powerful computers via the Internet. This raises concerns about who would be responsible if an accident occurred whilst a plant was being controlled, perhaps by another company or from another country, (Jones 1991). The advent of SCADA systems already allows this to happen but no accidents have so far occurred to test the legal position. Fraga and Laing point to the Internet as a means of making data available to a wide audience, (Fraga and Laing 1995). They illustrate the use of hyper-text documents in the épée environment for this purpose. Preston sees the future as intelligent, integrated process systems, (Preston 1996).

A currently rapidly expanding field is the use of portable machines but these suffer from problems of short battery life and poor quality displays. Their use can be expected to expand as communication channels become more readily available.

Expert systems have moved from the AI field into process engineering and it is expected that neural networks will make the same leap. Neural networks offer the advantages of being parallel devices for compatibility with advances in computer architecture. of having the ability to extract information from data efficiently and of minimising the need for first principles modelling. The application of other AI techniques to process design is also likely to occur. Modi and co workers consider the use of SOAR, with mechanisms of exhibiting intelligent behaviour, including

learning, for design, (Modi et al 1995). The ability of such systems to integrate multiple sources of information and apply them at the correct time is key. The promise of reduced design costs and reduced errors are held out as the benefits. Fraga and McKinnon acknowledge that lack of availability of parallel computers and similar machines is a barrier to the solution of large problems, such as integrated synthesis, (Fraga and McKinnon 1995). They propose that a network of more commonly available workstations could be used to exploit the under utilised computing power but point out that high communication times, and costs, could be a draw back for this approach.

Chapter 3

Market Survey

3.1 Introduction

When commencing the development of computer tools that are intended as aids to the process designer a number of factors should be considered:

(i) It is important to understand both the design process and the needs of the target users to ensure that the tools developed will be useful and supportive.

(ii) Any limitations imposed by the software and hardware platforms available to the users have to be acknowledged and the tools developed within these limitations. An element of crystal ball gazing is necessary to prejudge the changes that will occur during the development period.

(iii) To avoid wasting time and effort by reinventing the wheel for every new tool envisaged, knowledge of existing systems is necessary. Wherever suitable elements and precedents exist these should be utilised.

The understanding of the design process is addressed in Chapter 4 with the other factors being addressed by a market survey which is discussed here.

3.2 Development of software

There are four main routes by which process design software can be produced:

(i) The modification of commercially available base tools to carry out chemical engineering calculations. Spreadsheeting software such as Lotus 123 is the most commonly used base. Relatively simple calculations such as control valve sizing and line sizing can easily be tackled but for complex calculations the spreadsheet formate rapidly becomes cumbersome.

(ii) Software developed from scratch within a company to address a need that cannot be fulfilled by commercially available software. This situation normally arises when the technology or material being dealt with is in someway unique. In-house development and subsequent support of the tools

requires a considerable manhour and cost commitment. To protect commercial advantage this type of tool usually remains within the originating company. There are exceptions such as the ICI developed simulator FLOWPACK that was available to others.

(iii) Software originating in research programmes undertaken with or without industrial involvement in an university environment. Many of the current simulation tools, ASPEN, GEMS, SpeedUp etc, originated in this way. Generally a software house becomes involved in the final preparations for release onto the market place such as debugging.

(iv) Software developed by specialist software houses to fulfil an identified gap in the market. To recoup the costs involved in bringing such tools to the market the purchase costs are usually very high.

Reese argues that, based on Chevrons experience, the in-house development of any required software by a centralised computing provision allows standardisation, ease of communication and cuts the cost of both development and support, (Reese 1989). Most companies have now moved away from this position due to the overheads drain that such a centralised provision represents. Emerging data exchange standards have solved the problem of communication between tools from a variety of sources.

3.3 Available tools

Since 1989 Chemical Engineering Progress have published annual software directories giving extensive listings of tools available for all aspects of process plant design. These directories represent a fairly comprehensive picture of the commercially available software including basic information on the systems required to run it and the capabilities. As such they can be used to gain some of the background knowledge on available tools called for in section 3.1, point iii and to identify trends in both the type and capabilities of these tools. Other sources of information are the reviews published by Hydrocarbon Processing and the Chemputers feature included in Chemical Engineering.

3.3.1 Trends from the CEP Software Directories.

Five of the annual software directories published by Chemical Engineering Progress were analyzed to determine if any trends in the provision of software tools to Chemical Engineers could be uncovered, (C.E.P. 1990, 1991, 1992, 1993 and 1994). Due to the scope of the directories, the 1995 directory had over 1,500 programmes, it was not possible to review all the tools included and attention was focused on simulators. This focus is somewhat confused by the alteration, in the 1995 directory, of the classification categories used. The "Process Design / Simulation" category has been taken as equivalent to the earlier "Flowsheet Simulations" category. Table 1 compares the number of entries into the flowsheeting section over the years along with the number of software houses involved.

Table 1 - Flowsheeting Tool Quantity Trends.

Directory Year	Published Year	Number of Entries	Number of Contributors
1991	1990	25	17
1992	1991	41	27
1993	1992	40	25
1994	1993	55	29
1995	1994	125	72

Whilst the general trend appears to be in a steady increase in the number of tools offered the figures include many tools that, upon closer examination of the descriptions provided by the suppliers, do not conform to the generally accepted definition of a simulator. Taking this factor into account the figures for the number of simulators reported are as follows:

1991 (16), 1992(29), 1993(27), 1994(44), 1995(58)

The large leap in the 1995 directory cannot be relied upon for trend prediction due to the reclassification that occurred. Of the 58 tools identified as simulators 18 appeared in the 1994 directory under different classifications, indicating a more realistic comparison figure of 40. The major players in the simulation field have

maintained a consistent presence, with a varying product basket, whilst others tend to come and go. Concentrating on the major companies and the tools included in the market survey reported in Section 3.4.

In the 1991 directory the position was as follows:

Aspen Technology offered ASPEN PLUS (v8)

Simulation Sciences offered ASPEN/SP, PRO/II (v3.01) and PROCESS

ChemStations offered ChemCAD II (v2.4)

ChemShare offered DESIGN II

Hyprotech offered HYSIM C (v1.2)

Sacda offered MASSBAL (v2.0)

PPS Systems offered MASSBAL C

Prosys Technology offered SpeedUp (v5.2)

By the 1992 directory the position had not altered significantly from the above with the exception of the removal of Prosys Technology, and hence SpeedUp, from the listing. Hyprotech, Aspen Technology and ChemShare included new versions of their software, with the latter including a Windows based tool for the first time.

In the 1993 directory the position had become:

Aspen Technology offered ASPEN PLUS (v8.5) and SpeedUp (v5.3)

Simulation Sciences offered ASPEN/SP and PRO/II (v3.1) but not PROCESS

ChemStations offered ChemCAD II (v2.6)

ChemShare offered various versions of DESIGN II

Idaho Research Foundation offered GEMS for the first time

Hyprotech offered HYSIM (v2.0)

Sacda offered MASSBAL (v2.0)

PPS Systems offered MASSBAL C

The 1994 directory saw the removal of ChemShare, and hence DESIGN II. Other changes were a new version of ChemCAD by ChemStations, a new version of PRO/II by Simulation Sciences and the first mention of HYSYS by Hyprotech.

Revised classifications in the 1995 directory produced the following picture:

Aspen Technology offered ASPEN PLUS (v9.1) and SpeedUp (v5.4)

ChemStations offered ChemCAD III (v3.1)

Simulation Sciences offered PRO/II (v4.0 Win) but not ASPEN/SP

SEL-Hyprotech offered FLARESIM for the first time

Idaho Research Foundation offered GEMS

Hyprotech offered HYSIM (v2.0) and HYSYS

Sacda offered MASSBAL (v3.0)

Of the 24 tools mentioned during the market survey 16, ASCEND II, AutoCAD, AUTOPLANT, CADAS, FLARENET, FLOWMASTER, FLOWPACK, FLOWTRAN, HTFS, HTRI, PDS, PIPESIM, PDMS, QUASILIN, TECJET and ZYQUAD, do not occur in the simulation section of the C.E.P directories. Of these 8, ASCEND II, CADAS, FLOWPACK, FLOWTRAN, HTRI, PDMS, QUASILIN, and ZYQUAD, did not occur at all in the, indexed, 1995 directory with the remainder occurring in other sections. AutoCAD, AUTOPLANT and PDS appeared in the CAD/CAM Drafting section. FLARENET and FLOWMASTER appeared in the Fluid Dynamics, Particle Dynamics, Flow Analysis section. HTFS appeared in the Network Optimization: Heat Exchanger, Separation section. PIPESIM appeared in the Petroleum/Gas/Energy Production section. TECJET appeared in the Reliability, Failure Analysis, Risk Analysis section. The eight unmentioned tools fall into a number of categories. References for ASCEND II and QUASILIN are academic in nature indicating that these tools may not have yet reached the commercial market place. CADAS was developed in Norway and may not have penetrated the US market covered by C.E.P. FLOWPACK and FLOWTRAN were developed by commercial organisations, ICI and Monsanto respectively, over 20 years ago and are no longer actively supported as commercial tools. HTRI programmes were produced by an American company but the current status is unclear. PDMS is a 3-D modelling tool produced by a UK company that may not have significant penetration into the US market. ZYQUAD is in development with a group of consortium members and is not yet available for commercial release.

The C.E.P. Directories contain information on the hardware requirements, operating systems, peripherals and features of the programmes included. Examining this information over the years allows certain trends to be highlighted. These are discussed in the following sections.

3.3.1.1 Operating Systems. Software has been adapted to run on the various operating systems as they emerge. For ASPEN PLUS 386/AT with DOS appeared for the first time in 1992 followed in 1994 by 486 with DOS and in 1995 by Pentium with DOS. ChemCAD and HYSIM were a year earlier with DOS versions for 386's and 486's and started to offer Windows versions in 1994. Additionally HYSIM offers OS/2 and Mac versions giving it a very wide range of possible platforms. Workstations with Unix and mainframes have maintained a continuing presence. Not all tools are oriented towards the PC user, MASSBAL moved completely away from PCs in 1995 when a new version was released. SpeedUp is also predominantly Workstation based but offered a 486 with DOS version in 1995. PRO/II falls into a similar category but includes Windows versions for 486s and Pentiums.

3.3.1.2 Memory. The RAM required has shown an increase with a suggested figure of 8 MB now being common for process simulators, although ChemCAD only requires 640 kB. Trends for minimum hard disk size are less clear but generally show a peak around 1992/93 followed by a significant decline. In all cases the trend follows the release of new versions of the tools.

3.3.1.3 Display. Following the availability of display types the general trend has been away from Monochrome and EGA towards VGA and SVGA, with some tools continuing to support them all. SpeedUp is the exception, only offering an unspecified "other" display type.

3.3.1.4 Peripherals. Whilst, surprisingly, a mouse continues to be listed as an optional peripheral for many simulators the Maths Coprocessor has become a requirement in most cases. A wide range of other optional peripherals, such as modems and tablets, are supported in many cases.

3.3.1.5 Output Devices. No great changes in output devices are apparent over the period covered. Laser Printers, Postscript Printers and Plotters are all commonly supported. Dot Matrix and Ink Jet Printers continue to be supported in some cases.

3.3.1.6 Data Format. Other than proprietary formats specific to each tool the most commonly occurring data formats are ASCII and WK1. The use of proprietary formats is on the increase which causes concern over tool integration.

3.3.1.7 Other Features. The availability of help to the user in various forms, on line, hotline, training etc, is offered by all tools as are security features. One

significant trend is evident, the appearance of network versions in 1994 and 1995 as a response to the increased use of LANs.

3.3.2 Hydrocarbon Processing Reviews.

Less comprehensive reviews, focusing on design, simulation and optimisation tools for the refinery and petrochemical industries are published by Hydrocarbon Processing, (Hydrocarbon Processing 1994 and 1996). In 1994 56 applications were included with brief descriptions of application and capabilities. The presentations hinge on various hydrocarbon industry processing units and many of the tools discussed are applicable to a single unit type. The categories used, and the number of tools within each, are as follows: Distillation (5), Alkylation (4), Crude Unit (4), FCCU (4), Energy Integration (3), Hydrotreating (3), Olefins (3), Ammonia (2), Catalytic reforming (2), Dehydration unit (2), Delayed coker (2), Ethylene furnace (2), Refinery (2), Amine plant (1), Aromatics extraction (1), Cogeneration (1), Complex heat exchangers (1), Cooling water networks (1), Crude preheat train (1), Distillation thermodynamics (1), Gas sweetening (1), Glycol / Methanol injection (1), Hydrocracking (1), NGL recovery / stabilization (1), Nitrogen rejection unit (1), PET (1), Solvent dewaxing (1), Styrene (1), Sulphur plant (1), VCM furnace (1) and Visbreaking (1). As a comparison in 1996 66 applications were mentioned, split as follows: Crude Fractionation (7), Distillation (7), FCCU (7), Catalytic Reforming (6), Olefins (6), Alkylation (4), Hydrotreating (4), Dehydration (3), Gas Sweetening (3), Sulphur Recovery (3), Delayed Coking (2), Ethylene Furnaces (2), Hydrocracking (2), Hydrogen Plants (2), Styrene (2), Ammonia Plants (1), Heat Exchanger Networks (1), Natural Gas Processing (1), PET (1), Refinery Planning (1) and VCM Furnaces (1). As expected the most commonly occurring processing units with a high potential for economic impact occur most frequently, more so in the later survey. Given that the hydrocarbon industry was at the forefront of using computers in process design it is interesting to analyse the type of tools included. The split was as follows in 1994:

(i) 19 applications of more general simulators demonstrating a particular capability. Of these, six involved PROSIM, four ASPEN PLUS, two DESIGN II, two NOVA, two SPAN, two PRO II and one SpeedUp.

(ii) 14 tools are simulators for specific plant types.

(iii) 5 tools for off line simulation and optimisation of a specific unit type, with optional on line capabilities.

(iv) 4 tools for thermodynamic performance analysis.

(v) 3 tools for on line / real time optimisation and advanced control.

(vi) 2 dynamic simulators with trouble shooting and operator training capabilities.

(vii) 2 tools for non-linear modelling.

(viii) 2 tools for production scheduling.

(ix) 1 tool for plant data collection and off line optimisation with an option for use on line, for advanced control.

(x) 1 simulator capable of on and off line use including optimisation.

(xi) 1 off line optimiser.

(xii) 1 real time dynamic simulator.

(xiii) 1 tool for neural network model building.

The split was as follows in 1996:

(i) 19 applications of more general simulators demonstrating a particular capability. Of these five involve PRO/II and PROSIM, four HYSIM and HYSYS, four AKTIF, three NOVA and three PROSIM.

(ii) 15 tools for the off line simulation and optimisation of a specific unit type with optional on line capabilities.

(iii) 7 tools for on line / real time optimisation and advanced control.

(iv) 6 knowledge-based simulators with on and off line capabilities.

(v) 5 dynamic simulators with trouble shooting and operator training capabilities.

(vi) 4 tools for on line modelling with data reconciliation.

(vii) 4 tools for non linear modelling.

(viii) 2 tools for plant data collection and off line optimisation with an option for use on line for advanced control.

(ix) 2 simulators capable of on and off line use including optimisation.

(x) 1 tool for thermodynamic performance analysis.

(xi) 1 tool for production scheduling.

Whilst the degree of fragmentation, along the lines of unit type, exhibited is high the inclusion of on line, real time and dynamic capabilities in many of the tools indicates an encouraging degree of maturity in this field. The addition of knowledge based tools and the rise in the number of real time applications between 1994 and 1996 indicates advanced methodologies beginning to penetrate the commercial software market. However the appearance of knowledge-based elements in some tools points to a continuation of innovation. Given the selective nature of the handbook preparation it would not be valid to attempt to draw conclusions on trends from this data.

3.3.3 Chemputers.

The Chemputers feature has been included in Chemical Engineering for a number of years and covers all aspects of the software tools available which may be applicable in the field of process engineering. As such, much of the information and discussion included is not of direct relevance here but reviews of specific tools are included. Only those reviews that include tools of interest are discussed here. In 1985 a PC based distillation modelling tool, Prosep I, and a suite of calculation methods, Process Engineering Software Package (PESP), were included, (Lipowicz 1985). PESP included relatively simple programmes for fluid flow, heat transfer and equipment sizing along with a unit conversion module and represents a more organised approach than the collection of, often self generated, programmes that the average process engineer accumulates on their PC. In 1988 a drafting tool with the ability to extract data from a spreadsheet, ShamrockCADD, a PID controller simulator, Process Plus, a batch distillation design and simulation tool, BASIS, a physical property database, DIPPR, and a slurry-handling design tool, Slurry!, were discussed, (Hughson 1988). In reviewing available simulation and process control programmes Egol mentions PROCESS, HYSIM C, the EQUI-PHASE series of four programmes, ASPEN/SP-386, SuperFLIC, CAPE and CONTROL:Manufacturing, (Egol 1989). The last three are concentrated in the area of control design, the EQUI-PHASE series covers phase behaviour and the others are simulation tools. The feature of PROCESS and ASPEN/SP-386 that is highlighted as significant is the flexibility to handle a wide range of problems and for HYSIM it is the ease of use that allows complex problems to be handled easily. In the following year Egol

covers a larger number of programmes in a very brief way, (Egol 1990). Many are for well defined tasks such as control valve sizing and pump calculations but the general simulator MASSBAL is included as an example of a low cost tool with extensive functionality. A similar approach is taken by Shearman in 1991 but with a focus on aiding users determine which tool would be most appropriate, (Shearman 1991). As well as functionality and purchase cost users are encouraged to consider "hidden" cost such as hardware and training. The simulators included are split into specific and general. Specific tools mentioned are SimTool (v3.2), for fluid-thermal systems, MASSBAL C and Steambal C, for stream material balances, Codas-II and PCS, for control system simulation, PRO/II, for heat and mass balancing and Reaction, for modelling reaction schemes. Subsequent development of PRO/II has made it a more general tool. The general tools are SES/workbench, with the capability to allow examination of alternative process structures, Witness, for modelling the manufacturing process and PD-Plus, Slamsystem and ASPEN PLUS, general process simulators. A number of molecular modelling tools are also discussed. Suites of programmes designed to increase productivity and enhance performance are reviewed by (Shearman 1992). Those included are Engineer's Aide, containing nine programmes for equipment sizing, TK Solver, an equation processor, Process Package, containing common applications such as relief valve sizing and financial analysis, Chempax, for managing the manufacture and distribution of chemicals, DADiSP, for data manipulation, Mathcad, for algebraic calculations, Texim Project, Project/2, Open Plan, Microsoft Project and InstaPlan, for project management. The impact of the Pentium processor and the Windows NT operating system, with 32 bit architectures, on the types of simulation that can be carried out using a PC is discussed by (Shearman 1993). Increased computational ability and speed lead to an increase in the complexity of problems, such as dynamic simulation, that can be tackled but unfortunately many engineers still do not have access to systems containing these elements. Basta also highlights Windows NT as a major contribution to the increased utility of PC based simulation tools, (Basta 1995). NT versions of PRO/II, Design II and HYSYS are mentioned.

3.3.4 Other Sources.

Reading through any chemical industry journal produces a large number of

advertisements for software tools which claim to be indispensable for the practising process engineer. By responding to these advertisements a considerable amount of literature on commercially available tools, from a range of software houses, was accumulated. This information is briefly reviewed below.

3.3.4.1 Suites of design programmes. Engineer's Aide, by ENSIM, is a suite of nine integrated programmes, primarily for equipment sizing but with some project management capabilities. Process Engineers' Toolbox, by ChemEng Software and Services Ltd, contains 16 of the process engineering programmes developed by ChemEng Software. As well as a simple simulator the contents include equipment design, control, economics and management routines. Chemical Engineers PC Toolkit, by P&I Design Limited, was developed for use in the fine chemical batch processing field, with an emphasis towards predicting emissions from batch operations. The integrated modules include scrubber design, dispersion modelling and relief and blowdown design. The Chemical Engineering Expert, by Systema, is a suite of over 100 Lotus 1-2-3 spreadsheets for carrying out chemical engineering calculations such as air duct sizing, condensate flashing and utility costs. INPRO, by MAI Consultants Ltd, is a suite of equipment and system sizing routines for oil and gas production facilities that is aimed at the feasibility and conceptual phases of design.

3.3.4.2 Simulators. ASPEN PLUS, by Aspen Technology, is a widely used general, steady-state, process simulation tool with a GUI for ease of use. Integration with SpeedUp widens functionality to include dynamic simulation. MAX is a less sophisticated version of ASPEN PLUS aimed at obtaining results quickly within a PC environment. ChemCAD III, by Chemstations, is similar in functionality to ASPEN PLUS and can be integrated with AutoCAD and Lotus SmartSuite. The same company also offer BatchCAD for modelling the reaction kinetics and dynamic heat and mass balances for batch, semi-batch and continuous reaction systems. ECLIPSE, by University of Ulster, is a PC based simulation tool for energy conversion processes that was designed to support the evaluation of alternatives. GEMS, by Idaho Research Foundation Inc, is simulator for the pulp and paper industry. Development started in the 1970s and has continued since, with a Windows version now being available. HYSIM and HYSYS, by SEL-Hyprotech, are

respectively a steady-state simulator and a dynamic plus steady-state simulator, the later being released in the summer of 1995. MASSBAL, by SACDA, is an equation based simulator that can undertake steady-state and dynamic simulation. METSIM, by Proware, is a steady-state and dynamic simulator with a focus towards metallurgical processes. PD-PLUS, by Deerhaven Technical Software, is a PC based steady-state simulator that does not include graphical interfaces but is relatively cheap and has a low memory requirement. PMSolver Flowsheet Toolkit, by Digital Analytics, is a simulator based on the companies simultaneous equation solver packages with a number of standard modules available to the user. PRO/II, by SimSci, is a widely used, general simulator that is available with a GUI, PROvision. SimSci also offer PROTISS, an integrated environment for performing dynamic and steadystate simulations.

3.3.4.3 Drafting tools. AutoCAD, by Autodesk, is a drafting tool that is available with 2D or 3D capabilities and has a number of possible add-ons to enhance performance. Autodesk also offer a number of other drafting tools, including AutoSketch, a Windows based CAD tool, and AutoVision, with animation capabilities. PROCEDE, by Cherwell Scientific, is a package for the production of flow diagrams and specification sheets, designed to be used by the process engineer not a CAD operator. CADSIM, by SACDA, is a drafting tool that can be used to prepare presentation quality P&IDs that can also be used as inputs to the MASSBAL simulator. Microstation, by Intergraph, is a drafting tool with 2D, 3D and visualisation capabilities.

3.3.4.4 Specialist tools. PICCADEE is a programme for the design of pneumatic conveying systems. BioPro Designer, by Intelligen, is a simulator developed at MIT for the design of biochemical process. ADVENT and SPLIT, by Aspen Technology, are synthesis tools, for heat exchanger networks and distillation sequences respectively. Environmental Simulation Program, by Davy International, is a simulator aimed at processes with complex chemical systems. Example applications are the removal of SO_2 from incinerator off gas and catalyst regeneration. EnviroPro Designer, by Intelligen, is a simulator for the design and evaluation of environmental processes. FLUENT, by Fluent, is a tool for analysing flow problems. HEADd, by HTFS, is a tool for the preliminary design of heat exchange equipment. It acts

as an initial tool prior to the use of the HTFS suite of detailed exchanger design tools. POLYRED, by SEL-Hyprotech, is a simulator for the analysis and design of polymerization systems. OPC*MAP and FAST-EST, by OPC Engineering, are tools for the design and estimation of offshore and onshore, respectively, oil and gas facilities. INplant, PIPEphase and HEXtran are tools offered by SimSci for multiphase flow, pipeline and heat transfer simulations respectively.

3.3.4.5 Databases. Chemical Information Systems offer a number of databases, with on line access, containing SHE information on chemical substances. AEA Technology offer a failure rate database, REDAT. Under the blanket name of Numerica TDS offer a suite of databases in the fields of physical properties and environmental impact. Included are the well known physical property packages PPDS and DIPPR. Comline Ltd offer a suite of programmes, primarily in the field of materials selection but also including PIPECALC, for pipeline design, and INSTRUCALC, for sizing valves and flow elements. Solutions Software offer a CD-ROM database of all the US SHE regulations.

3.3.4.6 Miscellaneous. The Separation Processes Service of AEA Technology offer a number of tools based on the expertise that they have developed whilst undertaking consulting activities. Examples are CYCLONE2, for the design of cyclones, and LEXSET, for the design of mixer settlers. HAZSEC and HAZTRAC, by Technica, are tools for the recording and tracking, respectively, of HAZOP studies. Hazard Manager, by AEA Technology, is also a HAZOP recording tool. HYCON, by SEL-Hyprotech, is a tool that aims to support the conceptual design of separation systems. Databases of experimental data and distillation separation technology are used as the basis. PDQ$, by PDQS Inc., is a tool for preparing cost estimates for equipment items based on process flow sheet data. Under the banner of HAZWARE PrimaTech supply a suite of programmes aimed at improving the quality and completeness of hazard analysis studies. These cover the performance of studies and reviews and document handling. PROSPECTOR, by Granherne, is a design and cost estimating tool for offshore oil and gas fields. REACT!, by UnitOPS Software, is a programme for computing the equilibrium composition of mixtures of chemicals. PROSIM, by Bryan Research and Engineering, is a simulator for use in oil refining. The same company also offer TSWEET which focuses on gas sweetening simulation.

Supertarget, by Linhoff March, is a HEN tool. ZYQAD, by Zyqad, is an integrated design environment to support the production of deliverables throughout the lifetime of a project.

Given the high number of tools available it is difficult for a user to obtain sufficient information to make an educated choice of the most appropriate tool for them. Cost is easy to use as a basis but functionality may be more important in the long run and cannot be thoroughly investigated without use of the software. Many software houses provide evaluation copies of tools to allow this to take place but often these do not have the full capabilities of the programme. Given the high cost of the majority of packages and the pace of developments, in both hardware and software, a certain amount of crystal ball gazing is required when purchasing software to ensure that it does not become redundant before pay back is achieved.

3.4 Questionnaire

When designing tools to aid the design process it is important to understand the expectations of those who will use the tools as well as the underlying process of design. The latter is discussed in Chapter 4 and the former has been addressed by carrying out a market survey. The survey was designed as a questionnaire largely using a "tick-the-box" format to minimise the time required for completion. The original aims in designing the questionnaire were:

(i) To gain an insight into the current industrial position regarding the use of design tools in a wide range sectors.

(ii) To obtain pointers as to the direction industry would like to see design tools moving.

As the design of the questionnaire became finalised additional aims were added. These were related to the hardware used, perceived trends in hardware availability, the link between software and hardware and the reasons for selection/development of the systems used. A copy of the questionnaire sent out is included at the end of this chapter, as Figure 1. Sections 1 and 2.1 were included to aid analysis and comparison of responses.

3.4.1 Questionnaire Targeting.

To produce a meaningful set of results the aim was to obtain two or more responses from each target area. A target area consists of a combination of sector of operation, question 1.1, and design activities undertaken, question 2.1.1. A matrix with the sectors as rows and areas of operation as columns was used to gauge the adequacy of the responses received.

In late October 1994 63 surveys were dispatched, 38 to specifically named people and 25 to a generic "Process Engineering Manager", to which 30 responses were received. The response rate of 47.6 % was higher than the expected 30 % which is an indication of the importance attached to this field within the process industry. It is interesting to note that the response rate for companies outside the UK, where a stamped addressed return envelope was not included, was significantly lower. As neither company or individual names appeared on the responses, it was hoped that the anonymity offered would increase the response rate and encourage respondents to be candid, it was not possible to chase-up specific responses. However analysing the background information section of the responses against the target matrix allowed obvious gaps to be identified and a second mailing of questionnaires was undertaken in an attempt to fill these. This second batch included 19 mailings, all but two of which were to the generic title, and produced 8 responses. The lower response rate, 42.1 %, than for the initial mailing is still above that expected but is likely to be due to the lower level of specific targeting and the lack of involvement of addresses with the Ecosse group at Edinburgh. The target matrix reflecting both mailing stages is given as Figure 2.

Those sectors of the target matrix where the number of responses fell below the target value of two are highlighted in bold italics on Figure 2. Of the 153 sectors 39, 25.5 %, fall into this category, with the majority, 31 (20.3 %) being accounted for by two industry sectors, Metal Processing and Public Utilities, and two design activities, new product development and process licence package production. The average figures are included to emphasise areas of strength and weakness. All but one activity type achieved an average in excess of 2, with the exception being process licence package production which could be viewed as a rather specialist field. New product development and design management produced the lowest averages above

two, both coming in under three. The averages for these activities were pulled down by industry sectors in the bottom half of the matrix that are outside the traditional process industry. Discounting "Other" category, five of these sectors, Metals Processing, Minerals Processing, Biotechnology, Public Utilities and Pulp and Paper, produced averages below two. Of these by far the weakest was Metals Processing which may be a side effect of the relatively low representation of non-UK companies within the responses received. The poor showing in some grids of the matrix was expected due to the incompatibility of the industry sector and design activity. For example it is to be expected that Contracting and Consultancy scored poorly under new product development as this activity is outside their core business area.

3.4.2 Analysis of Responses.

As a means of identification and quick reference each response received was given a sequential number and this is used throughout the analysis. Tables 2 and 3, included at the end of this chapter, summarise the basic information against each identification number. The questions included are reviewed in turn in the following sections.

Table 2 gives a summary of the process industry sectors that respondent companies are active in. Responses under the "Other" category were reassigned if they fell under the intended remit of a named sector. The high number of entries for some companies may be misleading if it is attempted to analyse this table . For example a Contracting company may have either ticked only Contracting or Contracting and all the sectors to which they service. The same comment could also apply to Equipment Manufacture and Consultancy. Without taking this into account the average number of sectors ticked was 2.7. If a judgement is taken on which responses may be affected by this, thought to be 24 and 35, the average drops to 2.3. When analysing the responses to other questions in the survey the information contained within Table 2 will be used to see if there are any differences between industry sectors.

Table 3 gives a corresponding breakdown for the other element of the target matrix, the design activities carried out. Reference should be made to the above discussion of the target matrix for trend identification. It would have been interesting

to have access to similar data from a decade ago to see if the common held perception of a shift in detailed engineering capabilities from operators towards contractors was borne out.

3.4.2.1 Company roles (Question 1.2). Table 4 gives a breakdown of this information.

Table 4 - Company Roles

Role	Respondents
Plant Operation	4, 6, 7, 8, 13, 14, 15, 16, 17, 19, 21, 22, 23, 27, 29, 31, 32, 34, 35
Process Licensing	5, 12, 13, 17, 19, 20, 23, 24, 30, 35, 37
Plant Design	1, 2, 3, 4, 5, 6, 9, 10, 11, 13, 14, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 33, 35, 36, 37, 38
Equipment Manufacture	5, 11, 12, 14
Plant Construction	10, 14, 24, 25, 26, 28, 33, 35
Other	31 (R&D), 33 (Contracting), 37 (R&D)

The most frequently occurring response was plant design, undertaken by 81.6 % of respondents, followed by plant operation, 50 %, process licensing, 29.0 %, plant construction, 21.1 %, equipment manufacture, 10.5 %, and other, 7.9 %. The average number of roles ticked is 2.0. Research and Development and Contracting were named in the "Other" category, with the latter really intending to be covered by plant design. Although only two instances of R&D occurred as this was not included in the questionnaire it is unlikely that this represents a true picture of the number of respondent companies in this area.

The seven respondents not ticking plant design are 7, 8, 12, 15, 16, 32 and 34. Other than including no contracting or consultancy companies these are spread across a number of industry sectors. With the exception of Respondent 12, each ticked plant operation alone but all ticked a number of design activities in Question 2.1.1. Different interpretations of the wording of the form are likely to account for this effect.

Somewhat interestingly the only respondent, 20, who was active in the Equipment Manufacturing sector alone did not see themselves as undertaking the

equipment manufacture role, plumping for process licensing and plant design instead.

The respondents for each role include a wide range of process industry sectors and design activities. The most comprehensive spreads are given by process licensing and plant design. With only one exception, 14, plant operation is not carried out by contracting or consultancy companies. The opposite situation exists for plant construction where all but one, 33, of the respondents is a contracting and / or consultancy company. Such a situation was expected.

3.4.2.2 Regions of activity (Question 1.3). Table 5 gives a breakdown of this information.

Table 5 - Regions of Activity

Region	Respondents
Central Africa	11, 14, 24
Northern Africa	5, 11, 12, 14, 16, 21, 22, 24, 37
Southern Africa	1, 5, 9, 12, 14, 24, 26, 31, 37
Central America	5, 12, 14, 19, 20, 22, 24, 31, 37
North America	1, 2, 3, 5, 6, 7, 10, 12, 13, 14, 16, 17, 19, 20, 21, 22, 23, 24, 27, 30, 31, 35
South America	2, 5, 6, 7, 12, 13, 14, 20, 21, 24, 30, 31, 37
Asia	1, 3, 4, 5, 6, 7, 9, 10, 12, 14, 16, 20, 21, 22, 23, 24, 26, 31, 37
Australasia	1, 2, 5, 6, 10, 12, 14, 16, 24, 31
Eastern Europe	1, 3, 5, 7, 9, 12, 14, 16, 19, 20, 21, 22, 24, 25, 26, 30, 31, 37
Western Europe	1, 2, 3, 4, 5, 6, 7, 10, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38
Far East	1, 2, 3, 5, 7, 9, 12, 14, 17, 20, 22, 23, 24, 25, 28, 30, 31, 37
Middle East	1, 3, 5, 7, 9, 10, 11, 12, 14, 16, 20, 21, 22, 24, 25, 26, 28, 30, 31, 37

Notes. Respondent 8 did not tick regions of the world but stated that they operate in 120 countries worldwide. Respondent 13 added a comment to indicate that sales offices operate worldwide. Respondent 15 provided answers applicable to a single

UK site of a large international company. Respondent 33 is based solely in the UK.

If the comment by respondent 8 is taken as including every region all but two respondents are active in Western Europe, the exceptions being 9 and 11. They are also absent from the next most popular answer, North America. Respondent 9 is a contracting organisation with a spread of regions that suggests a bias towards the oil industry. Respondent 11 has the most unusual spread of regions, being active in the neighbouring regions of Central Africa, Northern Africa and the Middle East. This is difficult to reconcile with some of the claimed industry sectors, particularly Pulp and Paper. The ranking of the regions is as follows:

Western Europe	94.7 %
North American	60.5 %
Middle East	55.3 %
Asia	52.6 %
Eastern Europe, Far East	50.0 %
South America	34.2 %
Australasia	29.0 %
Northern and Southern Africa, Central America	26.3 %
Central Africa	10.5 %

The high position of Europe reflects the fact that the majority of respondents where based in this region, but otherwise the positions are roughly as would be expected given the economic position of the regions and the relative state of development of their process industries. Only 3 respondents, 8, 14 and 24, claimed to be truly global, with the average number of regions of operation being 5.2. There are no obvious links between process industry sector and regions of operation.

3.4.2.3 Methods of carrying out design (Questions 2.1.2 and 2.1.3). Tables 6 and 7 give a breakdown of this information.

Table 6 - Method of Carrying out Design

Design Method	Respondents
In-house	1, 7, 8, 9, 10, 11, 12, 20, 28, 30, 36, 38
Contracted out	
Mixture	2, 3, 4, 5, 6, 13, 14, 15, 16, 17, 18, 19, 21, 22, 23, 24, 25, 26, 27, 29, 31, 32, 33, 34, 35, 37

Table 7 includes only those respondents who are in the "Mixture" category in Table 6.

Table 7 - Split between Design Methods

Respondent	Percentage In-house / Contracted out
2	80 / 20
3	Varies from case to case
4	80 / 20
5	90 / 10
6	20 / 80
13	50 / 50
14	90 / 10
15	See Notes
16	90 / 10
17	25 / 75
18	50 / 50
19	30 / 70
21	10 / 90
22	50 / 50
23	10 / 90
24	80 / 20
25	95 / 5
26	90 / 10
27	80 / 20
29	5 / 95
31	30 / 70
32	25 / 75
33	50 / 50
34	80 / 20
35	85 / 15
37	75 / 25

Notes. Respondent 13 gave a 50 / 50 split but added a comment to say that detailed design was normally contracted out after the initial design had been done in-house. Respondent 15 added comments to the same effect with initial design 100 % in-house and detailed design 80 % contracted out.

The twelve respondents claiming to carry out all design in-house come from a range of industry sectors, with contracting, consultancy and equipment manufacturing companies constituting two thirds of the group. For these sectors an emphasis towards in-house design is expected as design expertise is core business and a wide range of design activity types are included. Six respondents active in these sectors, 5, 14, 24, 25, 26 and 35, contract out design but in all cases the split leans heavily towards in-house design, the lowest being 80 %. Of the four other respondents carrying out all design in-house three, 7, 8 and 36, undertake a range of design activities, from feasibility studies to detailed design, and one, 1, carries out only front end package production. In this latter case, if it is assumed that some of the packages produced are progressed further, subsequent design work must be contracted out. Three respondents, 7, 8 and 12, ticking that all design is done in-house claimed not to fulfil a plant design role in question 1.1.2.

Those using a mixture of design methods can be split into three categories, those carrying out the majority of design in-house (46.2 %), those with an even split (23.1 %) and those relying heavily on external design effort (30.7 %). The first group contains twelve respondents including the six contracting, consultancy and equipment manufacturing concerns discussed in the previous paragraph. Respondents 2, 4, 16, 27, 34 and 37 make up the remainder of the group, with respondent 37 having the lowest proportion of in-house design, 75 %. There are no obvious trends in industry sector or design activity type. Group 2 has six members, if respondent 3 is included, showing a strong leaning towards the chemical industry. Only respondent 33, Waste Treatment, falls outside this area. All design activity types occur with an emphasis away from detailed design and towards design management. The final group has eight members, 6, 17, 19, 21, 23, 29, 31 and 32, with the design type split varying from 30 / 70 to 5 / 95. All members are plant operators, in a variety of sectors, for whom design would be a non-core business activity. In terms of design activities undertaken there is a strong emphasise on front end

activities, such as new product development and feasibility studies, and away from detailed design. Not surprisingly all carry out plant modifications.

No respondent was completely dependant on external design effort. This would represent a vulnerability that would not make good business sense. Many large operating companies have moved away from maintaining large design departments, that could be viewed as overheads, and a survey carried out 10 to 15 years ago may have given a very different picture.

3.4.2.4 Proportion of staff involved in design (Question 2.1.4). Table 8 gives a breakdown of this information.

Table 8 - Proportion of Staff involved in Design

Proportion	Respondents
0 - 0.25	1, 4, 6, 7, 8, 12, 13, 15, 17, 18, 19, 21, 22, 23, 29, 31, 32, 34, 36
0.25 - 0.50	5, 16, 28, 30, 33
0.50 - 0.75	9, 11, 14, 24, 26, 35, 37, 38
0.75 - 1	2, 10, 20, 25, 27

Notes. No answer to this question was provided by respondent 3. Respondent 27 indicated that the proportion would be different for other sites within the organisation that have an operational focus.

It was expected that the proportion of staff undertaking design within a contracting organisation would be high. Whilst no company from this sector gave a proportion in the lowest sector one, 30, did tick the 0.25 - 0.50 box, a surprisingly low figure. In addition to plant design this company also undertakes process licensing, which has to be supported by design but may account for the value given. Bearing in mind the comment made by respondent 27 only two respondents, 2 and 37, outside contracting, consultancy and equipment manufacturing have more than 50 % of their staff involved in design. Respondent 2 is identified as the engineering arm of a large operating company and it is suspected that 37 falls into the same category. Conversely only respondent 12, an equipment manufacturer, from the sector group expected to be design oriented gave an answer in the 0 - 0.25 category. The numbers of persons employed in fabrication and instillation may have produced

this. There appears to be no correlation between the design activities undertaken and the proportion of staff involved in design.

3.4.2.5 Software used (Question 2.2.1). Table 9 gives a breakdown of this information.

Table 9 - Design Software Used

Software	Respondents
ASCEND II	12
ASPEN	2, 3, 5, 6, 10, 12, 13, 15, 17, 19, 23, 24, 26, 36, 37
ChemCAD	6
DESIGN II	9, 12, 17, 28
FLOWTRAN	
FLOWPACK	13, 17, 37
HYSIM	1, 5, 6, 7, 9, 10, 12, 14, 16, 17, 18, 21, 25, 26, 28, 29, 37
PRO II	1, 9, 10, 12, 13, 17, 20, 21, 25, 26, 29, 30
QUASILIN	
SpeedUp	2, 5, 17, 23, 24, 26, 27, 28, 29, 31, 36, 37
None	32, 33
Other	1, 3, 4, 8, 11, 16, 17, 19, 22, 24, 25, 27, 34, 36, 38
Proprietary	1, 7, 20, 29, 35

Notes. 1) The packages named under "Other" were as follows. HTFS was named by respondents 1, 17 and 24. HTRI was named by respondents 3 and 24. PDS was named by respondents 4, 8 and 34. AutoCAD was named by respondents 11, 22, 24, 34 and 38. PIPESIM was named by respondent 16. FLARENET was named by respondent 16. MASSBAL was named by respondent 19. CADAS was named by respondent 19. GEMS was named by respondent 24. PDMS was named by respondents 24 and 27. FLOWMASTER was named by respondent 25. FLARESIM was named by respondent 25. TECJET was named by respondent 25. ZYQAD was named by respondent 27. SUPERTARGET was named by respondent 36. AUTOPLANT was named by respondent 38.

2) Respondent 13 added a note to indicate regional variation in tool usage, ASPEN being used in USA only, with PRO/II the major elsewhere and some

residual use of FLOWPACK.

3) Of the six simulators mentioned by respondent 17 additional information was provided on the usage of three. DESIGN II is being faded out and the use of PRO/II started up. There is only an interest in HYSIM.

Ten software packages were included in the questionnaire and a further 16 were named by respondents. Two packages included in the questionnaire, FLOWTRAN and QUASILIN, were not selected as used by any of the respondents. FLOWTRAN has probably fallen out of use due to the age of the code, initial development took place in the 1960s and the lack of recent development. This programme lives on as the basis for the initial development of ASPEN. QUASILIN appears in academic references as a dynamic simulator but does not seem to have made the crossover into industrial use. The remaining 24 packages show the following usage pattern:

HYSIM	17 (44.7 %)
ASPEN	15 (39.5 %)
PRO/II and SpeedUp	12 (31.6 %)
AutoCAD	5 (13.2 %)
DESIGN II	4 (10.5 %)
FLOWPACK, HTFS and PDS	3 (7.9 %)
HTRI and PDMS	2 (5.3 %)
ASCEND II, ChemCAD, PIPESIM, FLARENET, MASSBAL, CADAS, GEMS, FLOWMASTER, FLARESIM, TECJET, ZYQAD, SUPERTARGET and AUTOPLANT	1 (2.6 %)

The average number of packages used is 2.4, with the following distribution:

None or in-house	3 (32, 33, 35)
One	11 (4, 7, 8, 11, 14, 15, 18, 20, 22, 30, 31)
Two	6 (2, 3, 21, 23, 34, 38)
Three	12 (1, 5, 6, 9, 10, 13, 16, 19, 27, 28, 29, 36)
Four	2 (26, 37)
Five	2 (12, 25)

Only two respondents, 32 and 33, claim not to use design software, either commercially available or developed in-house. Respondent 35 uses only software developed in-house. There are no links between the industry sectors or design activities of these companies.

A total of eleven respondents use only a single design tool. Respondent 4, an operating site of a large fine chemicals company, uses only PDS, a drafting package, as a design tool. PDS is also the sole design tool used by respondent 8, a chemicals / polymers operator. Similarly respondent 11, a small process systems and equipment company, does not use any simulation software but AutoCAD is used for drafting. Otherwise design is done using either spreadsheets or old FORTRAN and BASIC routines. AutoCAD is also the sole design tools used by respondent 20, an equipment manufacturer. Respondent 7, an oil refinery operator, uses a single simulator, PRO/II, and in-house software. Other companies using a simulator as their sole design tool are 14, an operator and equipment manufacturer, who uses HYSIM, 15, a petrochemicals operator, who uses ASPEN, 18, a fine chemicals design organisation, who uses HYSIM, 20, an equipment manufacturer, who uses PRO/II, 30, a contracting organisation, who uses PRO/II and 31, a food processing operator, who uses SpeedUp. The full range of design types are carried out by those utilising a single tool, which should be perfectly possible if the necessary unit operations and physical properties are supported.

The multiple tool users do not fall into any obvious patterns. The four users with the highest number of tools each carry out a wide range of design types but so do users with only a single tool. The size of the company and the ability to purchase and support multiple tools may be a factor but this cannot be determined from the survey as company size was not explored. Certain combinations of simulation tools do occur sufficiently frequently to be worthy of mention. In eight cases out of twelve SpeedUp occurs in conjunction with ASPEN, both offered by Aspen Tech. In two further cases it is used in conjunction with HYSIM and in the remaining cases no other simulation tool is used. In nine cases out of twelve PRO/II is used by companies who also use HYSIM, whilst the overlap with ASPEN is restricted to five companies. The reason for this is not clear but may be related to dynamic

simulation. The partnership between ASPEN and SpeedUp provides dynamic capabilities, as does HYSYS, the companion programme to HYSIM. PRO/II does not have dynamic capabilities but offers a functionality that exceeds that of the steady-state version of HYSIM. The high position achieved by programmes with dynamic capabilities indicates an increased acceptance of the importance of carrying out this type of simulation.

The "big four" programmes in the survey are HYSIM, ASPEN, PRO/II and SpeedUp. One aspect that could challenge the position of the Aspen Tech tools is the lack of availability of versions that can operate under the 32 bit architecture of Windows NT. The rival programmes already have this feature but it is not expected for ASPEN until 1998.

3.4.2.6 Software selection (Questions 2.2.2, 2.2.3 and 2.2.4). Table 10 gives a breakdown of the reasons given for the selection of the software used.

Table 10 - Reasons for Software Selection

Reason	Respondents
Compatibility with existing software	6, 7, 8, 17, 23, 30, 31, 37, 38
Range of features offered	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14, 16, 17, 19, 20, 23, 24, 25, 26, 27, 28, 30, 31, 36, 38
Previous experience of software house	1, 5, 8, 9, 12, 21, 22, 25, 37
Price	10, 16, 24
Recommendation by other users	9, 20, 22, 28, 37
Other	1, 15, 18, 25, 29, 34, 38

Notes. 1) Reasons given under the "other" category are as follows: Respondents 1, 25 and 38 indicated that specific choices are often dictated by customer requirements. Respondent 15, an operating site for a large company, utilises the company standard software and hardware system. Similarly respondent 18, part of a large design organisation, utilises a company standard system. Respondent 29 named universality and integrity as the reasons. Respondent 34 selected their CAD system as the industry standard.

2) Respondents 11, 32 and 33 did not provide any answers to these questions.

3) Respondent 35 uses only in-house software therefore question 2.2.2 is not applicable.

The most popular reason for selecting software across all industry and company types is, unsurprisingly, the range of features offered. However twelve companies did not tick this option. Four, 11, 32, 33 and 35, did not provide any answers to this question as they did not feel it applicable. Four, 12, 21, 22 and 37, selected their software based on previous experience of the software house. Two, 15 and 18, use company standard software selected by others. Respondent 34 selected their software based on their perception of the industry standard. The final respondent, 29, stands out from all the others in naming universality and integrity as reasons for software selection. It is not clear exactly what was meant by this.

Compatibility with existing software and previous experience of software house tie as the second most frequently occurring reasons. The first was not used as a sole reason for choice by any respondent indicating a willingness by process industry sector companies to move away from established systems if design demands are better served by a new one. The second is used as a sole reason for selection by three respondents, 12, 21 and 22, which could indicate satisfaction with the functionality of existing tools or a case of "better the devil you know". Moving to a completely new tool base represents a considerable expense, in capital and staff training, which represents a considerable amount of inertia for most companies.

Recommendation by other users is not relied upon heavily as a reason for software choice, cited by only five respondents. It can be viewed as a supporting factor.

The least frequently occurring factor is price, which always occurs in conjunction with range of feature offered. This indicates that process industry companies are prepared to make considerable investments in the "right" design tools. High cost tools without any associated enhanced functionality would not be successful.

Nineteen of the respondents indicated that hardware considerations did not effect the choice of software but this can probably be better expressed, in the words of respondent 16, as hardware being purchased to suit the software but not affecting

the choice. Expressed in this way this overlaps with the seven, 1, 6, 13, 17, 18, 24 and 34, respondants who commented that the purchased software had to be capable of running on PCs. Respondent 6 qualifies this by saying that the choice of PC based software only applied to some users. Respondents 25 and 26 required that the software purchased had to be available in versions that could run on the hardware platforms that they had available. Respondent 22 was the only one to mention that the cost of the necessary hardware affected software choices. Respondent 37 required that the software be compatible with the flexibility of the hardware platform. Eight respondents, 5, 11, 19, 20, 32, 33, 36 and 38, did not provide an answer to this question.

Twelve respondents indicated that software requirements had no effect on the hardware used. It is assumed that someone within these companies did check that the hardware platforms available could run the software before it was purchased. Eleven respondents, 9, 10, 12, 14, 16, 17, 23, 24, 25, 26 and 37, commented that software set the hardware specification by requiring a certain speed and power of PC in order to produce runs within an acceptable time. Six respondents, 4, 6, 19, 28, 36 and 38, also cite software affecting the hardware platform but for a variety of reasons. These are: the need to have a UNIX system, some users selecting VAX or workstations to run the software of their choice, the need for DEC based hardware, workstations to run SpeedUp whilst others use PCs, a move from VAX to PCs when the DOS version of ASPEN arrived and hardware selected for process compatibility. Respondent 29 called for technical integrity during system selection. Respondent 22 stated that ease of use and training affected the hardware and software platforms used. For respondent 1 the hardware platform used is dictated by corporate policy. Six respondents, 2, 5, 11, 20, 32 and 33, did not provide answers to this question.

The overall impression gained is that process industry companies do not see the costs associated with purchasing hardware as a bar to providing design tools to their workers. This appears to be generally confined to networks of high specification PCs.

3.4.2.7 Tool feature utilisation (Questions 2.2.5 and 2.2.6). Only one respondent, 38 a consultancy firm using AutoCAD and AutoPLANT, claims to use all the features of the available software heavily. The rest focus in on discrete areas. By

far the largest group of respondents mentioned simulation and flowsheeting as used most frequently. Fourteen companies, 4, 6, 9, 12, 16, 17, 18, 19, 23, 24, 25, 27, 28 and 31, who gave this answer exhibit no discernable trends in either industry sector or type of design carried out. As a subset of respondents they include users of all but two software packages mentioned in the questionnaire, again giving no indication as to any trends in feature utilisation. Respondent 6 added a comment to highlight the use of mass and energy balancing within simulation. These activities were also mentioned by respondents 21 and 36, with 21 specifying retrofit and conceptual balances. Respondents 12, 17 and 24 tied in physical property calculations along with flowsheeting and simulation, whilst 7 and 13 mentioned them on their own. This frequency of mentions indicates the vital importance reliable physical property estimation has during design. On a similar theme respondent 37 names the used features as the ability of the software to handle user preferred physical properties and user defined models. Four simulation packages are used by 37. Also in the area of modelling respondents 1 and 6 highlight separation simulation and modelling as heavily utilised. Other discrete modelling features mentioned were rating or design checking of apparatus capacity, 3, and flash calculations, 36. respondent 14 names the broader category of process design and analysis. Process optimisation only gets a single mention, 29, as does thermodynamics. There are only two responses from outside the area of traditional process engineering. Respondent 8, a chemicals area plant operator, uses finite element analysis most heavily and respondent 22, a fine chemicals operator and designer, uses many piping related features such as isometric modelling.

Nine respondents, 4, 7, 9, 17, 22, 23, 27, 31 and 37, state that there are no features of the software used that they find unnecessary. The software used by these companies is fairly randomly scattered. On a similar note respondents 3, 12 and 13 indicate that not many features have been found to be unnecessary, stating that software would not have been selected if this had been the case. Three respondents, 8, 21 and 28, say that features have been found to be unnecessary but do not specify which. Only six respondents state specific features that they find unnecessary. Respondents 6, 14 and 19 highlight costing with both 6 and 19 saying that the reason for this is that the estimates produced are too poor to be relied upon. Respondent

14 also finds equipment sizing unnecessary within HYSIM which indicates, as they undertake detailed and equipment design, the use of other tools for this activity. Respondent 36 states that distillation is unnecessary in their case, they design food processing plants using ASPEN and SpeedUp. Only respondents 29 and 38 cite software implementation issues as unnecessary features, these are user unfriendliness and the duplication of menus.

Almost a third of respondents, 12 (31.6 %) to the questionnaire did not provide answers to these two questions. A further four, 1, 16, 18 and 25, did not provide any response regarding features considered to be unnecessary. Respondent 24 rather evade this question by simply stating that it was difficult to answer. No real conclusion can be drawn from these numbers as the absence of an entry could be meant to imply that there are no unnecessary features.

The general impression gained from the answers to these questions is that people are relatively content with the software that they have selected for use. As the people completing the questionnaires are those who are likely to be responsible for the selection of software there may be an inherent reluctance to criticise their own choices. A different picture may be obtained from individual users within each company.

3.4.2.8 In-house development of design tools (Questions 2.3.1, 2.3.2 and 2.3.3). All but seven, 4, 18, 22, 31, 32, 34 and 38, of the respondents have found it necessary to develop in-house software. Tables 11 and 12 summarises responses.

Table 11 - Functions of Design Tools Developed In-house

Function	Respondents
Small, specialised design tasks	1, 2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 15, 16, 25, 27, 28, 33, 35, 37
Discrete, frequently carried out tasks	1, 5, 6, 7, 9, 10, 11, 12, 14, 16, 17, 19, 20, 23, 24, 25, 26, 27, 30, 33, 35, 36, 37
Large scale design tasks	5, 6, 7, 10, 12, 16, 17, 19, 20, 25, 30
Other	21, 29

Notes. Response under "Other" are as follows. Respondent 21 developed software for pipeline simulation. Respondent 29 cites optimization and chemical

characterisation techniques as reasons for developing software.

The most commonly named function carried out by in-house software is the performance of discrete, frequently carried out tasks, which was ticked by 23 of the 31 applicable respondents, (74.2 %). Examples of this type of task are the sizing of pipes and pump calculations. Small, specialised design tasks were named by 20 (64.5 %) respondents, with large scale design tasks being mentioned by 11 (35.5 %). Only two respondents named functions outside the list given in the questionnaire. Respondent 21 citing software for pipeline simulation, which could fit into either of the top two answers, and respondent 29 mentioning optimisation and chemical characterisation. The majority of respondents named more than one function that is carried out by in-house software indicating that it had been necessary to develop a number of tools. Of those only giving a single reason six, 2, 3, 8, 13, 15 and 28, named small, specialised design tasks, five, 11, 23, 24, 26 and 36, discrete, frequently carried out tasks and two, 21 and 29, other specified tasks. There are no apparent trends across industry sectors or company functions.

Table 12 - Reasons for Tool Development

Reason	Respondents
Unable to find suitable commercial tool	1, 2, 5, 6, 9, 12, 13, 14, 15, 16, 17, 20, 21, 25, 27, 29, 30, 35, 37
Capable tools considered unsatisfactory	1, 6, 7, 14, 23, 28, 35
Available tools considered too advanced	14, 35
Available tools too expensive	3, 16, 23, 24, 25, 26, 33, 35, 36
Prefer to develop all software in-house	5, 11, 12, 19, 25
Other	7, 8, 10, 15

Notes. 1) Responses under "Other" are as follows. Respondent 7 indicated the need to develop software based on internal standards developed using experience not available to third parties. Respondent 8 mentioned the need to issue software to customers as well as to use it internally. Respondent 10 stated that software had been developed for the mainframe computer prior to simulators becoming available. Respondent 15 comments that the development of in-house software for specific applications is simple to do. Respondent 17 states that development was undertaken

because suitable commercial software could not be found at the time.

2) Respondent 3 added comments to the effect that available tools were only too expensive in some cases with the development of in-house tools generally driven by the need to cover all the requirements of specialised design tasks.

By far the most common reason for having to develop software in-house was that companies were unable to find suitable commercial tools. Nineteen respondents (61.3 %) gave this as a reason and in the case of ten, 2, 9, 13, 17, 20, 21, 27, 29, 30 and 37, this is the only reason given. On the same theme respondents 10 and 15 indicate that such development was found to be necessary in the past due to the lack of suitable tools and that the tools developed continue to be supported. Given that cost did not appear as a major factor in the selection of software (Question 2.2.2) it is interesting to see that the second most popular reason for developing software in-house is that available tools are too expensive. Nine respondents ticked this reason, with four, 3, 26, 33 and 36, using this as the sole reason. Perhaps there is a cut off linked to price and generality, with companies prepared to invest in design tools with a wide applicability but more reluctant to spend on tools that are likely to be less generally used. Seven respondents considered that the tools capable of the tasks needed were not satisfactory, with one, 28, using this as the sole reason for development. A tool could be considered unsatisfactory for a number of reasons, such as being difficult to use or providing solutions to only a sub-set of the required tasks. Only five respondents indicate that they prefer to develop software in-house, with two, 11 and 19, citing only this reason for development. Two respondents considered the available tools too advanced for their purposes, indicating that software vendors generally pitch their tools to meet the needs of the market or that the market adjusts it's perceived needs towards the tools available. Respondents 7 and 8 indicated that they developed software in-house to encapsulate expertise that they wished to use for their commercial benefit. This need will always exist.

The general picture given is that companies will only make the investment to develop software in-house if they cannot locate commercial tools to carry out well defined design tasks, at a reasonable price. For the majority the preference would appear to be not to have to undertake this function.

3.4.2.9 Development language (Question 2.3.4). Table 13 gives a breakdown of this information.

Table 13 - Languages used to Develop In-house Tools

Language	Respondents
FORTRAN	2, 3, 5, 6, 7, 8, 9, 10, 12, 13, 14, 17, 19, 20, 23, 25, 27, 28, 29, 30, 36, 37
C	12, 13, 19, 20, 23, 27
C++	6, 17, 30
ACSL	
Other	1, 3, 7, 10, 12, 13, 14, 15, 24, 26, 33, 35

Notes. 1) Information provided under the "Other" category is as follows. Respondents 1, 7, 24, 26 and 33 indicated that developed tools are spreadsheet based. Quick Basic was named by respondents 3, 12 and 14. Turbo Pascal was named by respondent 3. Basic was named by respondents 10, 15 and 35. In the case of respondent 35 the Basic is compiled to speed up execution. Pascal was named by respondents 12 and 13.

2) This question was not applicable to companies who do not develop software in-house, (4, 18, 22, 31, 32, 34 and 38)

3) Respondent 6 indicates that FORTRAN was utilised in the past but that recently C++ has been used.

4) Respondents 11, 16 and 21 did not provide an answer to this question.

Of the 31 companies who do develop software in-house the most popular choice of language with which to do this is FORTRAN, named by 22 (71.0 %). Nine of these respondents, 2, 5, 8, 9, 25, 28, 29, 36 and 37, do not use any other language. C and the enhanced version C++ have a combined total of nine users, six (19.4 %) for C and three (9.7 %) for C++, all of which also use FORTRAN. The final language included in the questionnaire, ACSL, is not used by any of the respondents but four other languages are mentioned, falling into two groups. Basic

and Quick Basic are used by three respondents each, with respondent 15 using Basic alone. Pascal and Turbo Pascal are used by a total of three companies, the split being two to one, in conjunction with other languages. Five respondents do not use programming to develop in-house software but rely on spreadsheet based systems, in four cases, 1, 24, 26 and 33, this is the sole method used. The use of spreadsheets is discussed in more detail in section 3.4.2.11.

Companies show a tendency to stick to established languages when developing tools. This is probably dictated by the pool of expertise available. There are no obvious similarities between companies operating in the same industry sectors or carrying out the same types of design.

3.4.2.10 Use of Spreadsheets (Question 2.3.5). Of the 38 questionnaire respondents only two, 8 and 34, stated that they do not use spreadsheets during the design process. Seven respondents, 3, 4, 14, 20, 22, 31 and 32, did not provide an answer to this question but the remaining 29 all answered this question positively. A wide variety of tasks are mentioned with comments on the extent of use ranging from very little, respondent 28, to extensively, respondent 36. One of the most commonly occurring uses mentioned by respondents is that of undertaking simple, routine and repetitive calculations. A total of nine companies, 2, 7, 10, 13, 17, 18, 25, 26 and 28, use spreadsheets for this purpose. By no means all the uses of spreadsheets could be described as simple calculations, with respondents 5 and 19 using them for simulations, but in general the ease of use of spreadsheets for defined tasks is one of the features that has lead to their wide scale adoption and use. Heat and mass balancing, particularly during the initial stages of a project, is mentioned by seven respondents, 2, 9, 11, 17, 18, 27 and 36. This focus on simple, preliminary evaluations is also emphasised by respondents 6, 7, 15 and 37. Other uses mentioned a number of times are costing (6, 36 and 37), data handling (19, 26 and 27), scheduling (24 and 33) and unspecified design tasks (1, 12, 24, 30, 33 and 35). Three respondents, 16, 21 and 23, indicate that spreadsheets are used at the discretion of the individual designer to carry out a range of design tasks. Respondent 1 additionally uses spreadsheets to provide a reporting mechanism. Other reported uses are to draw graphs, 27, for investigating multiple conditions applied to empirical chemical engineering equations, 29, for "what if" scenarios, 37, and databases, 38.

Only one respondent, 13, expressed concern over the level of spreadsheet usage saying that they were too widely used but some of the uses mentioned above would appear to be rather ambitious for a spreadsheet.

3.4.2.11 Current hardware (Question 2.4.1). Table 14 gives a breakdown of this information.

Table 14 - Hardware Utilised

Hardware	Respondents
PCs	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38
Mainframe and Terminals	3, 4, 5, 6, 7, 9, 13, 15, 16, 17, 18, 19, 24, 26, 29, 31, 36, 37
Workstations	2, 3, 4, 5, 6, 7, 8, 9, 10, 14, 16, 18, 19, 22, 23, 24, 25, 26, 27, 28, 29, 31, 37

Notes. 1) Respondents 13, 17 and 36 indicate that their use of mainframe and terminals is dying out.

All 38 questionnaire respondents currently use PCs, with 11, 1, 11, 12, 20, 21, 30, 32, 33, 34, 35 and 38, using only this hardware platform. The second most popular hardware type is workstations, used by 23 respondents, 60.5 %. A mainframe and terminal set up is used by 18 respondents, 47.4 %. Fourteen companies use all three platforms. Of the four companies, 13, 15, 17 and 36, who use both PCs and a mainframe and terminals three, 13, 17 and 36, added comments to indicate that they use of the latter platform is in decline. These respondents may soon join the group who use PCs only. The remaining nine companies, 2, 8, 10, 14, 22, 23, 25, 27 and 28, use both PCs and workstations. The users of workstations are spread across a wide range of industries but concentrated amongst those using the simulators ASPEN, HYSIM and SpeedUp, all of which are computationally intensive.

The PC has arrived with avengence and is being embraced right across the process industry, with mainframe and terminal set-ups correspondingly in decline. Any software developer ignoring PC compatible software limits their potential market

considerably. The number of companies using workstations shows a willingness to move towards more costly hardware to run the more power hungary programmes.

3.4.2.12 Current operating systems (Question 2.4.2). Table 15 gives a breakdown of this information.

Table 15 - Operating System Utilised

System	Respondents
DOS	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 14, 15, 16, 17, 21, 23, 24, 25, 26, 27, 28, 30, 31, 33, 34, 35, 36, 37, 38
WINDOWS	1, 2, 4, 5, 6, 7, 9, 10, 11, 12, 13, 15, 16, 17, 18, 19, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 35, 36, 37, 38
UNIX	4, 5, 6, 7, 8, 9, 10, 12, 15, 16, 18, 19, 20, 24, 25, 26, 27, 28, 37
Vax / VMS	2, 3, 5, 6, 7, 8, 13, 14, 16, 17, 19, 23, 26, 27, 31, 36, 37
Other	24, 30

Notes. 1) Respondent 17 mentions moving to Windows NT.

2) Respondent 24 names Prime.

3) Respondent 30 uses Novell Netware 3.11 on network

The widespread use of the PC noted in section 3.4.2.12 is reflected by the most commonly used operating systems. Windows is used by 32 respondents, 84.2 %, and DOS by 31, 81.6 %. Only respondent 20 does not use either of these systems, this company utilises only UNIX. A total of 19 companies, 50 %, use UNIX and all but three, 12, 15 and 20, are workstation users. Vax / VMS systems are used by 17 respondents, 44.7 %, of which 12 are mainframe and terminal users. Other named systems are Prime, respondent 24, and Novell Netware 3.11, respondent 30. The latter is used for network servers. There are no obvious trends based on process industry sector or type of design work undertaken. The trends are related to the hardware used.

3.4.2.13 System selection (Question 2.4.3). Table 16 gives a breakdown of this information.

Table 16 - Reasons for System Selection

Reason	Respondents
Evolution of previous system	2, 6, 7, 8, 9, 11, 13, 17, 18, 19, 21, 22, 23, 24, 26, 27, 31, 32, 33, 35
User preference	1, 4, 6, 7, 22, 38
Flexibility	1, 3, 6, 7, 9, 10, 18, 20, 30, 36, 37, 38
Ability to network multiple users	1, 2, 3, 6, 7, 8, 9, 13, 14, 15, 16, 17, 19, 20, 23, 25, 28, 29, 30, 31, 35, 36, 37
Other	12, 17, 30, 34

Notes. 1) Respondent 5 stated that this question could not be answered as multiple systems are used.

2) Respondent 12 selected the computer system primarily to suit the in-house specialised database system.

3) Respondent 17 took a strategic decision to develop PC and network capability.

4) Respondent 30 selected their computer system to minimise cost.

5) Respondent 34 stated that they selected their system to suit the industry standard.

The most popular reason for selecting the computer system used is the ability to network multiple users which was ticked by 23 respondents, 60.5 %. It is stated to be the sole reason by six companies, 14, 15, 16, 25, 28 and 29. This focus on the need to network users indicates a move towards a realisation that it is necessary for information to be exchanged electronically between users. Twenty respondents, 52.6 %, cite the evolution of a previous system as a reason for selection, with seven, 11, 21, 24, 26, 27, 32 and 33, only quoting this. This could mean that companies are highly satisfied with the systems that they have used historically or that there is a reasonably high level of inertia to moving towards new systems. Twelve companies looked for flexibility when selecting the system used, with respondent 10 only considering this factor. As flexibility could be taken to mean different things to different people it is difficult to comment on this. Six respondents, 15.8 %,

considered user preference during system selection but only one, 4, used this reason alone. Perhaps this is indicative of a general attitude that users will adapt to use whatever tools they are given. Only respondent 5 did not provide an answer to this question, stating that the use of multiple systems made this impossible.

3.4.2.14 System performance (Question 2.5). 21 respondents scored all six performance criterion listed in the question, a further eight, 3, 4, 10, 12, 18, 22, 28 and 29, provided partial responses which omitted those factors thought not to be applicable. Table 17 and 18 give a breakdown of this information, per aspect and per company respectively. Respondent 30 added a comment stating that the administration side of SimSci leaves a lot to be desired but did not feel qualified to comment in any more detail. Respondent 34 commented that they could not understand the question as any tool could be used well or badly. Seven respondents, 1, 11, 15, 20, 21, 25 and 32, did not provide any comment on this question.

Table 17 - System Performance Aspect Scores

Aspect	Mentions	Low	High	Average	S.D.
Safety	25	1	9	5.6	2.16
Economic Optimization	26	2	10	6.3	2.24
Plant Operability	26	1	9	5.6	2.10
Plant Constructability	24	1	10	5.0	2.75
Environmental Impact	21	1	8	4.6	2.25
Plant Maintainability	25	1	8	3.9	2.24

As all aspects were given scores across a large part of the range from unsatisfactory, 1, to excellent, 10, there is obviously no consensus within the process industry on system performance. On average, economic optimization is seen as most satisfactory, with a score of 6.3, followed by safety and plant operability, 5.6, plant constructibility, 5.0, environmental impact, 4.6, and finally plant maintainability, 3.9. This order reflects the evolution of design tools, which initially focused on basic plant design tasks, such as equipment sizing, before branching out into other areas. It can be postulated that the use of HAZOP techniques may be a reason for safety and plant operability achieving the same score. The standard deviation does not vary significantly between the different aspects.

Table 18 - System Performance Company Scores

Respondent	Aspects	Low	High	Average	S.D.
2	6	2	9	5.0	3.46
3	5	6	8	7.0	0.71
4	3	6	8	7.3	1.15
5	6	3	8	5.0	1.90
6	6	2	8	4.2	2.40
7	6	7	9	8.0	0.89
8	6	5	7	6.0	0.63
9	6	2	9	4.7	2.58
12	3	1	8	3.3	4.04
13	6	2	5	3.0	1.26
14	6	1	8	4.2	2.64
16	6	1	10	5.8	3.89
17	6	1	6	3.7	1.97
19	6	1	6	3.3	2.07
22	3	8	9	8.3	0.58
23	6	1	8	4.7	2.50
24	6	5	5	5.0	0
26	6	5	8	5.8	1.33
27	6	3	9	6.7	2.25
28	2	3	5	4.0	1.41
29	4	3	6	4.8	1.50
31	6	6	8	6.8	0.98
33	6	1	6	3.2	1.72
35	6	4	6	5.0	0.89
36	6	1	8	3.2	2.86
37	6	5	8	6.2	1.33
38	6	3	10	7.0	2.37

Respondents 10 and 18 are not included in Table 18 as they each only gave a response for a single aspect, economic optimization in both cases. Companies can be split into two main categories, those giving a narrow range of scores and those covering a wider range. If a narrow range is defined as a low / high gap of three or less there are 12 companies, 3, 4, 8, 13, 22, 24, 26, 28, 29, 31, 35 and 37, in the first group, each with a standard deviation of below 1.50. This group can be further sub-split into optimists and pessimists, the first giving an average score of above five. Seven respondents, 3, 4, 8, 22, 26, 31 and 37, can be viewed as optimists, with scores between 5.8, 26, and 8.3, 22. Respondent 22 is the most upbeat of all the companies. The pessimists within the narrow range group, 13, 24, 28, 29 and 35, have average scores of between 3.0, 13, and 5.0, 24 and 35. Respondent 13 is the most pessimistic company in the survey. The group of wide range companies consists of 15 respondents, 2, 5, 6, 7, 9, 12, 14, 16, 17, 19, 23, 27, 33, 36 and 38. All but four of this category are viewed as pessimists, using the criterion given above, with scores of between 3.2, 33 and 36, and 5.0, 2. The optimistic companies in this group are respondents 7, 16, 27 and 38, with scores of between 5.8 and 8.0. The view taken on performance is not linked to the industry sector in which the company is active.

The system performance aspects used in this question are related to the criterion for judging success discussed in Chapter 4. As the target for tool developers must to achieve an excellent score across the board there is significant room for improvement. Non-traditional tool areas such as maintainability, environmental impact and constructability have particular room for improvement.

3.4.2.15 Future hardware (Question 3.1). Table 19 gives a breakdown of this information.

Table 19 - Hardware for the Future

Hardware	Respondents
PCs	1, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 22, 23, 24, 26, 27, 28, 31, 33, 34, 35, 38
Workstations	1, 3, 5, 6, 7, 8, 9, 10, 18, 19, 22, 24, 26, 27, 28, 30, 31, 36, 37
Mainframes	3, 31

Notes. 1) Respondent 2 did not feel able to predict the future.

2) Respondent 3 sees the hardware used in the near future remaining unchanged but cannot predict further.

3) Respondent 6 sees a move to a mid-size Cray.

4) Respondents 20, 21, 25, 29 and 32 did not provide an answer to this question.

Whereas all respondents currently use PCs, refer to section 3.4.2.11, they do not all predict that they will be using PCs in the future. Of the eleven respondents who did not tick PCs as a platform for the future five did not provide any answer to this question preventing any conclusions being drawn about their vision and a further one did not feel able to comment. However the remaining five, 8, 19, 30, 36 and 37, are interesting in that they currently use PCs but see their future needs as being fulfilled by workstations only. The decline in mainframe usage noted by some when describing their current platform is more marked here with only two respondents, 3 and 31, seeing their use remaining. For respondent 3 this use is only predicted for the near future as they did not feel able to comment further.

Many of the respondents who see PCs as the future hardware platform mention that they will be networked. Increased power is likely to be necessary to cope with advances in software. This may be the reason that some respondents predict a move away from PCs to workstations. The most noticeable trend is the move away from mainframes.

3.4.2.16 Future operating systems (Question 3.2). Table 20 gives a breakdown of this information.

Table 20 - Operating System for the Future

System	Respondents
DOS	1, 3, 8, 31, 33, 37, 38
Windows	1, 4, 5, 6, 7, 11, 12, 13, 14, 16, 17, 18, 24, 25, 26, 27, 30, 31, 33, 34, 35, 37, 38
UNIX	6, 8, 9, 12, 19, 24, 27, 31, 36, 37
Vax / VMS	3, 23, 27, 31, 37
Other	23, 28

Notes. 1) Respondents 2, 10, 15, 20, 21, 22, 29 and 32 felt unable to give a prediction.

2) Respondent 3 saw the current systems remaining in use for the near future but was unable to provide any further predictions.

3) Respondent 23 mentions Chicago and Open VMS.

4) Respondent 28 expressed regret that they would be using Solaris.

The perception of the future of operating system use produces a significantly different picture to that given by the current usage pattern, see section 3.4.2.12. Given that nine respondents did not feel able to make predictions on this point it is difficult to make direct comparisons. Not withstanding this the use of the DOS and Vax systems is predicted to decline. The number of mentions for DOS drops from 31 to 7 and those for Vax / VMS from 17 to 5, which would give a reduction in each case even if all none respondents used these systems. There is also the possibility of a decline in the use of UNIX but this is not clear. In three cases, 9, 19 and 36, a move to using UNIX alone is predicted but conversely in seven cases, 4, 5, 8, 16, 18, 25 and 26, companies who currently use UNIX and Windows see themselves using only the latter in the future. Overall the picture appears to be predicting a significant shift towards dependence on the Windows operating system, with an inherent DOS base. Respondent 21 reinforced this by adding a comment that they would like to move to Windows but are being restrained by the need to maintain global IT continuity. The Windows operating system is currently run in a number of different forms, Windows for Workgroups, Windows 95 and Windows NT. Driven by Microsoft corporate policy the future must lie with Windows NT and any subsequent versions.

3.4.2.17 Additional features desired (Question 3.3). A wide range of answers to this question were received, ranging from the need for no additional features, respondents 2, 4, 5, 8, 11, 15, 16, 19, 20, 21, 22, 25, 32, 33 and 38, to too many to mention, respondent 12, with respondent 10 being unsure.

The most commonly occurring desire was to have a greater degree of integration between design tools in-order to improve data handling. This was mentioned by nine respondents, 1, 3, 13, 17, 18, 24, 26, 27 and 30. Respondent

13 mentions the impact of the STEP and PDXI initiative in this area, whilst respondent 26 sees Windows as having a contribution. Respondent 17 would like to see improved integration of steady-state and dynamic simulation and an integrated system for pressure relief. In a similar area respondent 14 would like to see an engineering database for project design and execution, such tools are already in existence but tend to have been developed in-house and not to be generally available on the open market. Respondent 26 also considers the use of a project design database and comments that electronic document management will allow efficient management and control of project documentation. An added advantage of such systems is seen to be that QA systems will be more effective. The requests by respondent 27 for options management and by respondent 28 for traceability of test cases could be fulfilled by such a system. Respondent 26 hopes that including a graphics capability may also lead to improvements in productivity. One aspect of the networking necessary to allow users to communicate with each other effectively mentioned by respondent 13 is that this has forced users towards a standard desktop PC, with special circumstances only allowing the use of other platforms such as workstations.

Another group of wishes are related to specific features of software. Respondent 6 would like to have a process synthesis tool for the early phases of design. Respondent 7 would like dynamic simulation but this facility is already readily available on the open market. A similar comment could also be made to respondents 36's request for a GUI for dynamic simulation. Respondent 28 wishes to have the ability to automate tasks that are frequently repeated. Respondent 34 requires an improved drawing library. Whilst not highlighting particular additional features respondent 35 would like more comprehensive design software, assumed to mean that they wish to see a larger number of design functions carried out within a single design package. More specifically respondent 37 wishes to be able to carry out environmental and safety assessments. The most interesting request for additional features is made by respondent 31 who requires affordable virtual reality for use on a network.

The final group of wishes are a mixed bag related to a number of different aspects. Respondent 9 wishes to have the plotting abilities of packages improved to

make them faster and more economic. The large reports produced by some simulation packages can certainly be a problem. Increasing the speed of packages is also important to respondent 27 but the link to the processing capabilities of the hardware platform used makes this difficult to judge in isolation. Respondent 23 would like a means of verifying the authority of the software used. The only respondent mentioning a wish related to hardware is 29 who requires increased reliability from their existing systems, hardware and software.

3.4.2.18 Formulation of computing policy (Question 3.4). Table 21 gives a breakdown of this information.

Table 21 - Responsibility for Formulating IT Policy

Authority	Respondents
Engineers	1, 3, 4, 5, 6, 8, 9, 10, 11, 12, 15, 16, 17, 19, 20, 22, 24, 25, 26, 27, 28, 29, 35, 36, 37
Systems Administration	2, 3, 4, 6, 10, 13, 14, 15, 16, 17, 19, 21, 23, 24, 25, 26, 27, 31, 32, 34, 36
Management	1, 3, 6, 7, 9, 16, 18, 19, 20, 24, 25, 26, 30, 31, 33, 35, 37, 38
Other	18

Notes. 1) Respondent 6 indicates that having three factions responsible for policy formulation can lead to conflicts.

2) Respondents 10, 15 and 19 state that Engineers formulate software policy. Hardware policy is determined by either management or systems administration.

3) Respondent 18 mentions that head office have a role to play in formulating policy.

4) Respondent 23 states that systems administration formulates software policy but that there is no single policy on software, resulting in variations from site to site.

5) Respondents 24, 25 and 26 have a special IT / Business improvement group, with a wide membership, to formulate policy.

Half of the companies rely on a single group to formulate IT policy. Of these

nineteen seven, 5, 8, 11, 12, 22, 28 and 29, depend on engineers, seven, 2, 13, 14, 21, 23, 32 and 34, depend on systems administration and the remaining five, 7, 18, 30, 33 and 38, utilise management for this role. Given the different perspectives on the problem that the different groups will have this situation is somewhat surprising. A more satisfactory approach would appear to be the IT groups mentioned by respondents 24, 25 and 26, all contracting organisations, where discussions can take place and a balance be struck between cost and functionality.

3.4.2.19 Additional Comments

A number of respondents added additional comments in the space provided, many of these related to clarification of company set up and answers given to specific questions which have been included above but there were a number of others that will be dealt with here.

The level of interest in this area is underlined by the number of respondents who expressed support for the aims of the questionnaire and indicated that they would be interested in the results. Respondent 14 highlighted a problem in this field in that developments are occurring so fast that answers to many of the questions will only remain valid for a short period of time. Comments on software and hardware use can only be taken to represent a snap shot at the time of completion. A concern raised by respondents 23 and 32 is that it is difficult for smaller concerns who do not carry out high levels of design to afford to buy tools with all the capabilities needed and to have them under utilised. Respondent 32 avoids the purchase, hardware and training costs involved by employing outside design agencies to carry out this work. Respondent 23 finds monitoring the quality of the software difficult, particularly when users have significant gaps between applications. Respondent 13 provided the highest number of comments. The company operates a number of small scale batch processes with complex chemistry and find that these dominate their selection of design software, with physical properties a particular problem. They would like to see university developed tools focusing on solving particular problems or on demonstrating application of novel principles or software techniques.

3.4.3 Tools mentioned in the Questionnaire.

Below is a brief discussion of the tools included in the market survey

questionnaire and those additional tools mentioned in responses.

3.4.3.1 ASCEND II

Included in the questionnaire. ASCEND II is an equation oriented simulator developed by Westerberg and co workers. It has dynamic and optimisation capabilities. The user interfaces with the programme interactively allowing the level of detail present in a run to evolve, (Locke and Westerberg 1983).

3.4.3.2 ASPEN

Included in the questionnaire. ASPEN is a sequential modular simulator with simultaneous modular convergence options but no dynamic capability. ASPEN was developed at MIT in the late 1970s, (Evans et al 1979), and due to lack of experience with the simultaneous modular architecture at the time was originally purely sequential modular. FORTRAN was used in the development to assist portability between platforms and due to the number of people familiar with this language. A preprocessor type structure is used where an input translator generates a programme that is then executed to perform the simulation. A large number of files are generated during an ASPEN run and these can subsequently be interrogated to gain information on the simulation. Current versions commonly utilise the Model Manager user interface, a GUI which is fairly user friendly, that has superseded the original free-format inputting style.

3.4.3.3 AutoCAD

AutoCAD, by Autodesk, is a PC based CAD tool that has been a market leader since the early 1980's. Release 13 appeared in late 1994. To remain attractive compared to expensive workstation based CAD packages additional features have been added over the years, including a move towards 3-D capabilities. Yares discusses Designer, a parametric feature-based modeller, that was first usable with AutoCAD 12, (Yares 1995). Designer includes solids modelling and constraint management capabilities.

3.4.3.4 AUTOPLANT

AUTOPLANT is an integrated suite of applications for the design and drafting of control systems, (C.E.P. 1994). It operates within the AutoCAD graphics environment.

3.4.3.5 CADAS

CADAS is a sequential dynamic simulator based on a distributed control system called AIM 1000 which was developed in Norway by SINTEF and Simrad Albatross, using government funding, (Naess et al 1993). It is object-oriented with the basic building block being a module that is represented by an algorithm defining actions. The development aim was the production of a tool for dynamic analysis over the whole life cycle of a project. CADAS was written in C to operate under UNIX with the graphical user interface implemented in X/Motif. Naess and co workers report the use of CADAS for stability analysis of an Ammonia synthesis reactor.

3.4.3.6 ChemCAD

Included in the questionnaire. ChemCAD is a flowsheet simulator which includes the capability to produce PFD quality graphics. Kernan reports the announcement by ChemStations of ChemCAD III including the ability to model electrolyte reactions, (Kernan 1993). The capabilities of the Tower+ module, to model distillation columns, within ChemCAD is discussed by (Lipowicz 1987). Whilst the module was slower than those it was compared with it was found to give reliable results.

3.4.3.7 DESIGN II

Included in the questionnaire. DESIGN II, by ChemShare, is a sequential modular simulator, with simultaneous convergence options for multiple recycle flowsheets, (Biegler 1989). It has dynamic capabilities to cover the modelling of systems such as batch distillation, with reaction and blowdown studies. DESIGN II was removed from the C.E.P. software directory in 1994 and is likely to gradually fall out of use, although Basta does mention work on a Windows version, (Basta 1995). An advertisement for this appeared in Hydrocarbon Processing in June 1996 claiming to be the first Windows simulator. Background information on a previous revision of the tool, DESIGN/2000, is given by (Matulsky 1982).

3.4.3.8 FLARENET

FLARENET, by SEL-Hyprotech, is a Windows based programme for the design and rating of flare headers based on user specified limits for noise, back pressure or mach number, (C.E.P. 1994). Multiple relief cases can be handled. A

database of components and pipe fittings is included.

3.4.3.9 FLARESIM

FLARESIM, by SEL-Hyprotech, is a programme for analysing thermal radiation from flares, (C.E.P. 1994). A 3-D analysis is carried out with optional modules calculating noise, surface temperatures and multiple burners.

3.4.3.10 FLOWMASTER

FLOWMASTER, by Flowmaster, is a one-dimensional internal flow analysis package to simulate gas or liquid flow in complex piping systems, (C.E.P. 1994). Steady-state and dynamic conditions can be handled. A graphical interface is used for data inputting and results presentation.

3.4.3.11 FLOWPACK

Included in the questionnaire. FLOWPACK was initially developed by ICI alone in the early 1970's and was used internally for five years before FLOWPACK II was developed in collaboration with the German contractor, Linde, (Berger and Perris 1979). FLOWPACK II was designed to provide a decade of flowsheeting capability for the two companies. ICI have subsequently taken a decision not to support further development to extend this life and have moved to the use of the commercial simulators ASPEN and PRO/II.

Whilst appearing to the user to be a sequential modular simulator FLOWPACK II has features that are simultaneous, (Biegler 1989), to overcome the potential inefficiencies in this approach. The basic sequential modular appearance was chosen by the developers as this represents the way in which users consider plants. Berger and Perris include examples to illustrate the range of possible uses for the initial version of FLOWPACK II, these are as follows:

(i) Interactive input for a simple reactor system balance.

(ii) Fertilizer granulation process to demonstrate solids handling capabilities.

(iii) The use of sub units to decompose a flowsheet and increase computational efficiency.

(iv) Complex heat exchanger networks to demonstrate the ability to handle bypasses etc.

3.4.3.12 FLOWTRAN

Included in the questionnaire. FLOWTRAN was developed by Monsanto in

the mid 1960's to pull together unit operation models that had been developed in-house. By 1969 it was marketed outside Monsanto and had built up a user base of approximately 70 across a wide range of industries, (Rosen and Pauls 1977). Outside Monsanto use has been mainly limited to the North American petrochemical industry. FLOWTRAN was used by MIT as the basis for the development of ASPEN. It is a steady-state sequential modular simulator.

3.4.3.13 GEMS

GEMS (General Energy and Material balance System), by Idaho Research Foundation, is a modular flowsheet simulation package for pulp and paper applications, (C.E.P. 1994). A combination of general flowsheeting blocks, eg MIX and REACT, and specific unit operation blocks, eg Kraft digesters, are used to build models.

3.4.3.14 HTFS

HTFS (Heat Transfer and Fluid flow Service) is a generic name for a suite of programmes for the design of heat exchange equipment produced in the UK under the auspices of the National Engineering Laboratory.

3.4.3.15 HTRI

HTRI (Heat Transfer Research Incorporated) produce a suite of heat exchange equipment programmes that are rivals to the HTFS suite.

3.4.3.16 HYSIM / HYSYS

Included in the questionnaire as HYSIM. The development of HYSIM is described by (Morris et al 1985). In early 1980 Hyprotech undertook a project to develop a process simulator that did not rely on batch processing, as programmes with roots in mainframes tend to, but was interactive. The approach adopted is described by Morris and co workers as programmable calculator based, with the simulator approaching a problem in a similar way to an engineer armed with a calculator. To facilitate this models need to be written in such a way that bidirectional and partial flows can be handled. Complexity, of the models, is increased as they have to be able to determine what variables are known and those that can be calculated from this data. The user can then input known information and the programme will, on screen, calculate as much of the other stream data as possible. An under specified problem will not the solvable. An over specified

problem results in warning messages. Between 1980 and 1983 HYSIM was available on a minicomputer timesharing service in the Calgary area. When the maths co-processor became commonly available in 1983 HYSIM was converted to run on IBM-PC but initially the size of the programme, 1.3 MB, caused problems as it exceeded the RAM of PCs. This caused rather cumbersome segmentation. HYSYS was introduced in 1995 to provide a tool that could undertake both steady-state and dynamic simulation.

The balance user interface employed by HYSIM / HYSYS is similar to that seen in mass balance calculations undertaken by spreadsheet. The data is presented in a tabular formate with recalculation occurring as soon as any variable is altered. This approach allows the user to see the impact of changes much more clearly and rapidly than the more usual method of preparing an input file that is then submitted for running.

Lipowicz provides an assessment of the distillation column simulation capabilities of HYSIM 3.5, using COLUMN, (Lipowicz 1987). Ease of entering the problem data and the ability to produce graphical output are highlighted as desirable features. The physical property options were however said to be somewhat limiting at the time.

3.4.3.17 MASSBAL

MASSBAL is a simultaneous modular simulator originally designed for the pulp and paper industry, (Shewchuk 1982), where the performance of other simulators was found to be unsatisfactory. One of the main reasons for this is the difficulty in defining the physical properties to be used. Example inputs and outputs from the first version of MASSBAL are included by Shewchuk. Subsequently the focus has broadened to cover a wider industry base. The implementation of the equation oriented approach to simulation used by MASSBAL is discussed by (Stephenson and Shewchuk 1986).

MASSBAL 3.0, with dynamic capabilities, was announced in 1993, (Kernan 1993), with the steady-state version, MASSBAL 2.0, being offered in parallel. It contains four modules:

(i) Massbal. A general heat, mass and momentum balance simulator.

(ii) Energy. For modelling of steam generation, steam distribution, steam

utilisation, condensate recovery and boiler feedwater systems.

(iii) Evap. Handling the concentration of industrial liquors and solutions.

(iv) Furnace. For modelling furnaces and boilers.

After the user has set up the process and selected the materials and equipment from the internal database dynamic simulation is achieved by adding events such as a valve closing into the simulation. MASSBAL 3.0 can run on mainframes, 386 PCs with Unix or OS/2 or Macintosh 2x machines. MASSBAL is written in C. In addition to the full simulators SACDA offer less sophisticated versions of MASSBAL for balancing operations.

3.4.3.18 PDS

PDS (Plant Design System), by Intergraph, provides an integrated environment for the production of drawings such as PFDs, P&IDs and Layouts, (C.E.P. 1994). 3-dimensional modelling can also be supported. The system uses a relational database to store the data related to a drawing and can be used to produce customised reports. Features include interference detection to eliminate construction problems and the automatic generation of bills of materials.

3.4.3.19 PIPESIM

PIPESIM is a multiphase flow modelling tool with system analysis capabilities, (C.E.P. 1994). It forms part of a suite of tools used in the oil exploration field.

3.4.3.20 PDMS

PDMS is a 3-D plant modelling tool by CAD Centre, (Sawyer 1993). Barton and co workers describe the use of PDMS during the design of an oil / gas production platform, (Barton et al 1986). The database management system included allowed "intelligent" use of the data for tasks such as interface checks, generation of isometrics and material take offs. Overall savings of at least 25 % of the cost of the total facilities engineering phase of the project were claimed to arise from the reduction in errors seen. The same saving was claimed by BNFL for the application of PDMS to the Thorp project, (Wheeldon 1992). Clash detection capabilities and a reduction in errors are highlighted as key factors.

3.4.3.21 PRO/II

Included in the questionnaire. PRO/II is a general process simulator introduced by SimSci in 1990 to replace PROCESS. It can operate under a Windows environment. Graphics for flowsheet building are provided by PROvision. PRO/II includes the ability to handle solids.

3.4.3.22 QUASILIN

Included in the questionnaire. QUASILIN is an equation oriented simulator with dynamic capabilities. It was developed in the late 1970s by a team at the University of Cambridge, (Gorezynski et al 1979). QUASILIN was initially only a steady-state simulator which was then modified to have dynamic capabilities, (Smith and Morton 1988). The structure of QUASILIN is that the unit modules return equations describing the units to the executive which then solves the set of equations describing the process. Linearised equations represent the operation of the units and the assembled set are solved by a modified form of Gaussian Elimination to give a set of process variables. The process is repeated until convergence occurs. Hutchinson and co workers report the performance of QUASILIN against six test problems, (Hutchinson et al 1985). Whilst successful runs were eventually obtained in all cases a tendency to fail if presented with a badly posed problem was uncovered.

3.4.3.23 SpeedUp

Included in the questionnaire. SpeedUp is an equation oriented simulator developed by Sargent and co workers at Imperial, initially marketed by Prosys Technology it is currently offered by ASPEN Tech. It has dynamic capabilities. Reported uses include design of a process heater, (Bouwens and Kösters 1992), and applications in the minerals processing industry, (Barton and Perkins 1988). The minerals processing industry has traditionally not been an area where simulation is used heavily. Solids-processing with a wide range of possible feed quality variations and poorly defined physical properties characterise this field and make it difficult to handle in most simulators.

Sawyer canvassed for opinions on the use of SpeedUp and reports usage by three companies, WS Atkins, BP Engineering and Air Products, (Sawyer 1991). The uses included studies of compressor behaviour, transient behaviour of flare systems

and modelling of pressure swing adsorption processes for gas separation. All users were reported to be pleased with the performance of the package.

3.4.3.24 SUPERTARGET

Although the technique of pinch analysis is now commonly accepted the application to real plants has tended to remain the preserve of specialist consultants. Part of the reason is the cost of the software necessary to carry out such analysis. SUPERTARGET by Linnhoff March, a leading consultant in this area, is such a tool. The average process engineer will only undertake such analysis when a cheaper tool is available. Kemp mentions such a tool, HERO, available in a Windows format at a cost of about £200, (Kemp 1995).

3.4.3.25 TECJET

TECJET, by DNV Technica, is a package for modelling continuous jet releases, (C.E.P. 1994). It is designed to handle the full range of conditions and parameters that occur in real jets and includes a database of over 60 chemicals.

3.4.3.26 ZYQUAD

ZYQUAD is the name commonly used to refer to the Process Workbench tool marketed by ZYQUAD. It is an integrated environment, using expert system technology, designed to support the design process. The focus is on the intelligent production of design deliverables, such as PFDs and specification sheets, making use of all the prior knowledge accumulated by a company.

3.5 Conclusions.

The level of responses to the questionnaire received indicates that there is a wide ranging interest in the use of computer based design tools within the process industry. This has meant that it has been possible to achieve the aims of gaining an insight into the current software and hardware position and obtaining pointers for the future. A generally good spread of responses against the target matrix was achieved, with weaknesses in the Metal Processing and Public Utility sectors and in the product development and process license package production functions. All design activity types are well represented. There is a reasonable world spread but with a focus on Europe.

For the tools mentioned the most commonly used are HYSIM, ASPEN,

PRO/II and SpeedUp. When selecting the tool to be used functionality and the ability to network far out weigh cost, but cost does become important if the scope of application is limited. A high proportion of companies have found it necessary to develop software in-house to address specialised and discrete tasks when suitable commercial software could not be found or was too expensive. The majority would prefer not to do this. Spreadsheet usage is wide spread and they undertake many different functions. PCs with Windows are the most commonly used platform and are likely to remain so in the future, supplemented by workstations for power users. Networking is seen to be important as a means of system selection and as an area where improvements could be made. This ties in with the need to improve the integration of tools and allow data handling to become more efficient.

There is room for significant improvement in the performance of design tools against the six criterion for judging success. With particular attention required against maintainability, environmental impact and constructability.

The lowest response rate achieved was for questions 2.2.5 and 2.2.6, which examined the utilisation of software features. Almost a third of respondents failed to provide answers. Whether they did not do so because they felt it would disclose more information than was acceptable or because they simply did not know, is unclear.

Computer Based Design Facilities Questionnaire

This questionnaire forms part of a study into both the current and projected use of computers in process industry related design. It is being undertaken as part of our research programme in Integrated Process Design at the University of Edinburgh.

The ultimate goal of this work is better chemical processes through better design, where design encompasses the whole range of activities carried out by engineers to improve the final product.

The main purpose of this questionnaire is to gain background knowledge of the computer based design facilities currently used by companies operating in different sectors of the process industry and undertaking different types of design. It is also aimed at developing an understanding of the facilities that the industry would like to have available.

In an attempt to reduce the time needed to complete this questionnaire the questions have been presented in the 'tick the box' formate wherever possible. A small amount of space has been allowed for responses that do not fit into any of the given categories but if you wish to make extra comments please provide these on the blank sheet of paper provided making a note of the questions to which they relate.

Some of the questions are deliberately open ended to allow you to provide as much, or as little, information as you wish.

1 Background Information

1 What sector(s) of the process industry is(are) your company active in ?

Sector	Tick
Oil Exploration	
Oil Refining	
Petrochemicals	
Fine Chemicals	
Pharmaceuticals	
Food Processing	
Agrochemicals	
Waste Treatment	
Metal Processing	
Minerals Processing	
Biotechnology	
Public Utilities	
Pulp and Paper	
Contracting	
Equipment Manufacture	
Consultancy	
Other - Please specify	

2 What role(s) does your company undertake ?

Role	Tick
Plant Operation	
Process Licensing	
Plant Design	
Equipment Manufacture	
Plant Construction	
Other - Please specify	

3 What regions of the world are your company active in ?

Region	Tick
Central Africa	
Northern Africa	
Southern Africa	
Central America	
Northern America	
Southern America	
Asia	
Australasia	
Eastern Europe	
Western Europe	
Far East	
Middle East	

2 Current Facilities

2.1 Design Work Undertaken

1 What design based activities does your company carry out ?

Activity	Tick
New Product Development	
New Process Development	
Feasibility Studies	
Front End Package Production	
Detailed Design	
Equipment Design	
Process Licence Package Production	
Plant Modifications	
Design Management	

2 How are these design activities carried out ?

Method	Tick
In-house	
Contracted out	
Mixture of the above	
Other - Please specify	

3 What percentage of design work falls into each of these categories ?

Method	%
In-house	
Contracted out	
Other	

4 What proportion of staff are involved in design based activities ?

Proportion	Tick
0 - 0.25	
0.25 - 0.50	
0.50 - 0.75	
0.75 - 1	

2.2 Commercial Design Software

1 Which industry specific design software does your company use ?

Software	Tick
ASCEND II	
ASPEN	
ChemCAD	
DESIGN II	
FLOWTRAN	
FLOWPACK	
HYSIM	
PRO II	
QUASILIN	
SPEEDUP	
None	
Others - Please specify	

2 Why was the software used selected ?

Reason	Tick
Compatibility with existing software	
Range of features offered	
Previous experience of software house	
Price	
Recommended by other users	
Other - Please specify	

3 Did hardware considerations influence the choice of software ? If so how ?

4 Conversely did software considerations influence the choice of hardware ? If so how ?

5 What features of the commercially available design tools used are most heavily utilised ?

6 Are there any features of these tools that are considered to be unnecessary ?

2.3 Other Software

1 Has your company found it necessary to develop in-house design tools ?

Yes No (circle as appropriate)

2 What functions do any tools developed perform ?

Function	Tick
Small, specialised design tasks	
Discrete, frequently carried out tasks	
Large scale design tasks	
Other - Please specify	

3 Why was the development of these tools required ?

Reason	Tick
Unable to find suitable commercial tool	
Capable tools considered unsatisfactory	
Available tools considered too advanced	
Available tools too expensive	
Prefer to develop all software in-house	
Other - Please specify	

4 What language was used to write these tools ?

Language	Tick
FORTRAN	
C	
C++	
ACSL	
Other - Please specify	

5 Are spreadsheets used during the design process ? If so what function do they fulfill ?

2.4 Hardware

1 What hardware does your company use ?

Hardware	Tick
PC's	
Mainframe and terminals	
Workstations	

2 What operating system do you use ?

System	Tick
DOS	
WINDOWS	
UNIX	
Vax/VMS	
Other - Please specify	

3 Why was the current computer system selected ?

Reason	Tick
Evolution of previous system	
User preference	
Flexibility	
Ability to network multiple users	
Other - Please specify	

2.5 System Performance

How would you rate, on a scale of 1 (unsatisfactory) to 10 (excellent), the overall performance of the design tools and computer system available to you with respect to the following aspects of design ?

Aspect	1	2	3	4	5	6	7	8	9	10
Safety										
Economic Optimization										
Plant Operability										
Plant Constructability										
Environmental Impact										
Plant Maintainability										

3 Future Facilities

1 What hardware do you see your company using in the future ?

2 What operating system do you see your company using in the future ?

3 What additional features would you like to see added to your current design environment ?

4 Who within the company is responsible for formulating policy towards software, hardware and operating systems ?

Authority	Tick
Engineers	
Systems Administration	
Management	
Others - Please specify	

Additional Comments

Table 2 - Process Industry Sectors

Response No.	Process Industry Sector(s)
1	Oil Refining
2	Fine Chemicals, Other (Fibres and Coatings)
3	Petrochemicals
4	Fine Chemicals
5	Oil Refining, Petrochemicals, Pharm., Biotechnology, Equip. Manufacture
6	Oil Exp., Oil Refining, Fine Chemicals, Agrochemicals, Other (Polymers and Fibres)
7	Oil Refining
8	Fine Chemicals, Pharm., Agrochemicals, Other (Polymers)
9	Contracting
10	Contracting, Consultancy
11	Fine Chemicals, Pharm., Food Processing, Waste Treatment, Minerals Processing, Pulp and Paper, Equip. Manufacture
12	Oil Exp., Oil Refining, Petrochemicals, Fine Chemicals, Pharm., Waste Treatment, Pulp and Paper, Equip. Manufacture
13	Fine Chemicals, Pharm., Food Processing, Agrochemicals, Waste Treatment, Minerals Processing
14	Contracting, Equipment Manufacture, Other (Gas and Cryogenic)
15	Petrochemicals
16	Oil Exp.
17	Oil Refining, Petrochemicals, Fine Chemicals
18	Fine Chemicals
19	Oil Exp., Petrochemicals, Pharm., Agrochemicals, Metal Processing, Public Utilities
20	Equip. Manufacture
21	Oil Exp.
22	Fine Chemicals, Pharm., Other (Detergents)
23	Petrochemicals
24	Petrochemicals, Fine Chemicals, Pharm., Food Processing, Agrochemicals, Waste Treatment, Minerals Processing, Biotechnology, Pulp and Paper, Contracting, Consultancy
25	Contracting
26	Contracting
27	Other (Nuclear Power)
28	Oil Exp., Oil Refining, Food Processing, Waste Treatment, Consultancy
29	Oil Exp.
30	Contracting
31	Food Processing, Other (Research)
32	Pharm.
33	Waste Treatment
34	Waste Treatment
35	Oil Refining, Petrochemicals, Fine Chemicals, Pharm., Food Processing, Waste Treatment, Contracting, Consultancy
36	Food Processing
37	Other (Gas Production and Processing)
38	Consultancy

Table 3 - Design Activities Undertaken

Response No.	Design Activities
1	FEPP
2	NProdD, NProcD, FS, DD, PM
3	DD
4	NProdD, NProcD, FS, FEPP, DD, ED, PM, DM
5	NProcD, FS, DD, ED, PLPP, PM
6	NProdD, NProcD, FS, FEPP, PM
7	FS, FEPP, DD, PM, DM
8	NProdD, NProcD, FS, DD, ED
9	NProcD, FS, FEPP, DD, PM
10	NProcD, FS, FEPP, DD, ED, PM, DM
11	ED
12	NProdD, NProcD, FS, FEPP, DD, ED, PLPP, PM
13	NProdD, NProcD, FS, FEPP, PM, DM
14	NProcD, FS, FEPP, DD, ED, DM
15	FS, PM, DM
16	FS, FEPP, DD, PM
17	NProdD, NProcD, FS, FEPP, DD, ED, PLPP, PM, DM
18	NProdD, NProcD, FS, FEPP, DD, PM, DM
19	NProdD, NProcD, FS, DD, ED, PM
20	FS, FEPP, ED, PM
21	NProcD, FS, FEPP, PM, DM
22	NProdD, NProcD, FS, FEPP, DD, PM
23	NProdD, NProcD, FS, FEPP, PLPP, PM, DM
24	NProcD, FS, FEPP, DD, ED, PM, DM
25	NProcD, FS, FEPP, DD, ED, PLPP, PM, DM
26	FS, FEPP, DD, PM, DM
27	NProcD, FS, FEPP, DD, ED, PM
28	NProcD, DD
29	NProcD, FS, FEPP, PM, DM
30	NProcD, FS, FEPP, PLPP, PM
31	NProdD, NProcD, FS, PM
32	FS, FEPP, DD, PM, DM
33	FS, DD, PLPP, PM, DM
34	NProcD, FS, DD, ED, PM, DM
35	NProdD, NProcD, FS, FEPP, DD, PM, DM
36	NProcD, DD, PM
37	FS, DD, PLPP
38	FEPP, DD, ED, DM

Key to Table 3

NProdD - New Product Development
NProcD - New Process Development
FS - Feasibility Studies
FEPP - Front End Package Production
DD - Detailed Design
ED - Equipment Design
PLPP - Process Licence Package Production
PM - Plant Modification
DM - Design Management

Figure 2 - Completed target matrix

	B1	B2	B3	B4	B5	B6	B7	B8	B9	AVE
A1	3	6	6	5	4	2	*1*	6	2	3.9
A2	4	6	6	6	6	3	3	6	3	4.8
A3	8	9	10	6	8	5	4	10	5	7.2
A4	9	10	10	8	9	6	2	9	6	7.7
A5	6	8	9	6	8	6	2	8	4	6.3
A6	3	6	4	3	4	2	*0*	5	3	3.3
A7	4	5	5	3	3	3	*0*	4	2	3.2
A8	3	6	6	4	6	4	2	6	5	4.7
A9	*1*	*1*	*1*	*0*	*1*	*1*	*0*	*1*	*0*	*0.7*
A10	*1*	2	2	2	*1*	2	*0*	2	2	*1.6*
A11	*0*	2	2	*1*	2	2	*1*	2	*1*	*1.4*
A12	*0*	*1*	2	*1*	2	*1*	*1*	*1*	*0*	*1.0*
A13	*1*	2	2	2	2	3	*1*	2	*1*	*1.8*
A14	*1*	7	8	8	7	4	2	7	6	5.6
A15	*1*	3	4	3	3	5	2	3	*1*	3.8
A16	*1*	4	3	4	5	3	*0*	3	4	3.0
A17	*1*	2	2	2	2	*1*	*0*	*1*	*1*	*1.3*
AVE	2.8	4.7	4.8	3.8	4.3	3.1	*1.2*	4.5	2.7	

Key to Figure 2

A1 - Oil Exploration
A2 - Oil Refining
A3 - Petrochemicals
A4 - Fine Chemicals
A5 - Pharmaceuticals
A6 - Food Processing
A7 - Agrochemicals
A8 - Waste Treatment
A9 - Metal Processing
A10 - Minerals Processing
A11 - Biotechnology
A12 - Public Utilities
A13 - Pulp and Paper
A14 - Contracting
A15 - Equipment Manufacture

A16 - Consultancy
A17 - Other
B1 - New Product Development
B2 - New Process Development
B3 - Feasibility Studies
B4 - Front End Package Production
B5 - Detailed Design
B6 - Equipment Design
B7 - Process Licence Package Production
B8 - Plant Modifications
B9 - Design Management

Chapter 4

Hierarchical Design Methods

4.1 Existing Models of Process Design

Although there is an extensive body of literature concerned with the modelling of chemical plants, and consequently many tools developed to undertake the mechanics of the design process, relatively little has been published concerning the modelling of the process by which the design takes place. To deal with this aspect requires a move away from the traditional mathematically based approach to chemical engineering design in order to encompass more abstract concepts and thought patterns. The field of artificial intelligence has already developed techniques to address many of the issues and provides a source of methods that can be adapted for use in providing intelligent support to designers.

Before such support can be provided it is necessary to identify what is to be supported, i.e. to develop a valid representation of the design process. There have been a number of different models proposed over the years with varying levels of complexity. At a very basic level the onion diagram (Linnhoff et al 1982, Lott 1988) can be said to be such a model. The elements of a chemical plant are represented in a ring type structure with the reactor at the centre working out through separation and heat integration to utility systems. Inherent in this representation is the assumption that design will commence with the design of a reactor system and proceed in an orderly manner until all the ancillary items have been specified. Other than this implication the onion diagram does not model the design process or attempt to address the way in which an engineer would approach a design problem, this is perhaps inherent in a model that is based on a simple representation of the relationship between physical processes.

A more sophisticated model is the hierarchical structure due to Douglas (Douglas 1988), which is discussed in greater detail in the following sections. This attempts to model the way in which an engineer would tackle a design, i.e. to systemize the procedural knowledge that is used during design. The basis of this

method is outlined in (Douglas et al 1985). It follows the commonsense approach to process design which starts at a relatively abstract level and adds successive levels of detail as the design progresses. The hierarchy originally proposed by Douglas has subsequently been refined, (Douglas 1992), to increase the range of applicability and broaden the factors considered. Douglas and Stephanopoulos claim that the basic hierarchy requires only minor modification to cover processes with solids, polymer processes, biochemical processes and batch processes, (Douglas and Stephanopoulos 1994). As discussed in section 4.2.2 this statement is somewhat misleading as the Douglas technique suffers from the drawback of a lack of generality. Such a characteristic is identified by Douglas and Stephanopoulos as an important feature of a hierarchical decision procedure. As it is obviously not possible to use information that has not yet been produced the design development must follow the flow of information, hence it would be difficult to argue against the validity of some form of hierarchical model of the design process. Such a structure mirrors the way in which process engineers tackle a design problem and hence the approach does not represent any fundamental progress in the understanding of the design process. The work by Douglas does represent one of the most comprehensive attempts to systemize the procedures involved in design into a series of steps that can be easily followed and applied to the users design. As observed by Tanskanen et al there is an inherent danger that the creativity necessary for design will be stifled by the use of a design methodology in the form of a sequence of tasks with associated heuristics to support decision making (Tanskanen et al 1995) and it could be argued that the Douglas approach exhibits this characteristic. However to develop a useable model systematization is necessary with the skill and experience of the engineer undertaking the design being a more significant factor in the creative content. The hierarchical models presented by Douglas are very much unit operation based.

One of the prime reasons for developing a model of the design process is to allow computer based tools to be developed that will aid the designers. Smithers et al argue that in order to provide intelligent support to designers it is necessary to go beyond simply building programs that exhibit behaviour similar to that of a designer, such as those models mentioned above, and explore the generation, use and organisation of knowledge (Smithers et al 1990). This argument requires a model

which stretches beyond looking at the mechanics of the design process and covers the field of knowledge management. The exploration-based model of design is proposed to address the requirement (Smithers and Troxell 1990). Bañares-Alcántara builds on this work in the development of the KBDS system, which is discussed in Chapter 6 (Bañares-Alcántara 1995), but also points out that the use of a hierarchical design model is of fundamental importance to the development of a representative model of the whole design process. The conclusion that can be drawn from the above is that for the development of a support tool for design it is necessary to consider models for both the procedures involved in design and for the use of knowledge. This is the basis for the phenomenon driven process design methodology developed by (Tanskanen et al. 1995).

The focus in this chapter is on developing a realistic model of the procedures involved in design, i.e. modelling the approach that an engineer would take to process design. The development of a support tool for the design process will be discussed elsewhere. A hierarchy is the most logical and realistic model of the approach and that due to Douglas represents the greatest formalisation of this model. As such the Douglas hierarchy forms the best basis for the development of a model that addresses the short comings within it. The base hierarchy (Douglas 1988) is briefly outlined in the next section followed by a discussion of points of contention, some of which have been at least partially addressed by (Douglas 1992). A case study is used to illustrate these points and finally an alternative hierarchical model is proposed.

4.2 The Douglas Hierarchical Method

The basic principle that under pins the approach to conceptual process design due to Douglas is to get something down on paper as quickly as possible and use this initial design as a basis for subsequent refinement and optimisation. To achieve this end extensive use is made of heuristics, to speed the decision making process, and a basic hierarchy of five decision levels was developed. The five levels for petrochemical processes containing only vapour/liquids are briefly described below and reference should be made to (Douglas 1988) for a more detailed description. This reference also contains information on the modification of the basic hierarchy

for application to both solid processes and batch processes. These modified hierarchies contain additional steps, one in the case of the solids hierarchy and two for the batch hierarchy.

Level 1. Here the basic information required for the design is collected and the only decision to be taken is the choice between batch and continuous plant. The rest of the method applies only to continuous plants.

Level 2. At this level the process is treated as a black box with inputs and outputs and the decisions to be taken all relate to the number of each of these that there should be. Specifically the destinations of feed impurities and by-products are considered.

Level 3. This level is concerned with the reactor system and decisions to be taken cover aspects such as number of reactors, ratios of reactants, choice of reactor conditions to achieve the desired conversion and heat transfer requirements.

Level 4. Initially at this level the general structure of the separation system is determined by looking at the phase of the reactor effluent. The system is then split into two parts, termed the vapour recovery system and the liquid separation system, for further consideration. The decisions to be taken are different for the two parts, concentrating on type and location of system for the vapour recovery section and primarily on distillation for the liquid separation section.

Level 5. At the final level the well known techniques of heat integration, as developed into a commonly used tool by Linnhoff and co-workers at UMIST (Linnhoff and Flower 1978), is applied to the flowsheet previously developed.

This basic structure of levels generally follows the pattern of information flow through a design and therefore represents a relatively logical model format. However there are a number of major points of contention, with both the structure and the principles underlying it, that are discussed below. Some of these are then illustrated by the application of the Douglas approach to a published case study of the manufacture of MEK from 2-Butanol (Austin and Jeffreys 1979). Although a rather trivial point the naming of the levels is misleading at times which may lead to

confusion over intent. Specifically Level 3 would be better termed "Reactor System" rather than "Recycle Structure" to reflect the decisions involved. Also the naming of the vapour section of Level 4 as "Vapour Recovery System" rather than "Vapour Separation System" presupposes that the plant product will be liquid rather than gas phase, usually but not always, the case.

There is no direct link between the levels proposed by Douglas and the phases of design identified in Chapter 2. As a design methodology Douglas is concerned with phases 1 to 4 only with a heavy emphasis towards phases 1 to 3 rather than towards phase 4, detailed design. During phase 1, feasibility studies, it is unlikely that the design of any of the options under consideration would progress past level 2 although there may be some attempt to produce preliminary PFD's. All five levels may be considered during phase 2, conceptual design, with the extent of detail developed being dependant on the time available and the number of options being considered. Fully developed P&IDs would only be developed for one route during phase 3, front end design, and hence it could be said that the conclusion of level 5 only occurs at this point.

The modified structure proposed by (Douglas 1992) contains eight levels but due to the lack of information contained within the paper about levels 5 through to 8 it has not been possible to use this as a case study basis. Levels 1 to 5 represent the basic structure described above with the addition of points to address waste handling in particular. The basic thrust of the approach being to consider the destination of all streams and to carefully consider the impact of any additional streams introduced by unit operations. It would also appear that an increased amount of attention is paid to safety factors and that solids processes have been incorporated, Level 4 contains an additional subdivision to address this. Levels 6, 7 and 8 are termed evaluation of alternatives, flexibility and control and safety respectively but no further details are provided. Table 1 gives a summary of the models proposed by Douglas. Douglas first addressed the need to address solids processes in conjunction with Rossiter, (Rossiter and Douglas 1986). They presented an alternative six level hierarchy for these systems that could only be used for solids systems and could not consider unit operations handling more than one solids processing step. This restriction precludes the inclusion of items such as spray dryers. Rajagopal and co

workers describe the modifications to the basic Douglas hierarchy to allow solids to be handled, (Rajagopal et al 1992). In addition to the five basic levels a sixth is added for the evaluation of alternatives. At level 1 the only change is the need to indicate product, by product and feed stream phases. These are key in determining separation system structure at Level 4. Level 2 also remains virtually unchanged although there are additional possibilities for feed purification. Level 3 is modified to add decisions related to the handling of solids around the reactor e.g. is a melter or dissolver required before the reactor. At Level 4 the phase separation step becomes more complex with three phases (vapour-liquid-solid) and an additional sub-level is needed to handle solid separations. Levels 5 and 6 were not utilised fully in the study reported. There are a number of limitations on applicability that severely restrict the use of the method. Namely: only one primary product can be handled, vapour-solids processes cannot be handled and only low molecular weight solids can be handled. Further restrictions apply to the computer implementation, in PIP, due to model limitations. Another alternative, containing seven levels, is given in (Douglas and Stephanopolous 1994). This adds one stage, input information, to the start of the basic five stage procedure and one, creation and evaluation of alternatives, to the end. Level 4 is further sub split into seven stages: General separation structure, vapour recovery system, solid recovery system, liquid separation systems, gas separation system, solid separation system and combined separation system. This enables a broader range of plants to be tackled than previously but leads to a high degree of fragmentation. Whilst reducing the separation synthesis problem into "bite size" chunks there is the danger of moving towards a situation where it is not possible to find the optimal solution to the overall problem. Other modifications have also been proposed by Douglas over the years. These are discussed where relevant in the sections below.

4.2.1 Generation of Alternatives

During process design, particularly the feasibility study and conceptual design phases, there are many issues that cannot be fully resolved. These issues may arise for one or more of a number of reasons, with commonly occurring reasons for uncertainty at the early stages being:

(i) Inability to define a project specification until some design work has been undertaken.

(ii) Poor availability of basic design information, with the lack of adequate physical property data usually being a problem.

(iii) Lack of design methods and models that are known to be applicable.

(iv) Inability to predict market conditions.

These and all the other issues that could equally well be named as sources of uncertainty are all due to one root cause, the absence of unambiguous knowledge. Whatever the reason for the existence of uncertainty the resultant unresolved issues can cause severe problems with the design process. At one extreme a single design path is pursued until a dead end is reached causing an inability to progress any further along that path further. To restart the design process it is necessary to backtrack along the path until a decision point is reached that gives access to an alternative path. Any design that involves a significant amount of such backtracking from a number of dead ends entails the wasting of effort and inefficiency. Even if a single pass approach to design did not result in any dead ends it is highly unlikely that the resultant design would be even close to optimal. It is worth noting however that a complete pass through all the stages of design would be necessary to resolve and rank some of the alternatives generated. This point is discussed further when looking at the alternative model proposed. Looking at the other end of the spectrum where high levels of uncertainty exist it is possible to become bogged down in so many different possible design routes that progress effectively ceases. This is also highly inefficient. All real designs contain uncertainty and therefore the potential for either of these scenarios making the generation of alternatives and the need to manage them properly are an integral part of design. The ideas expressed here can be summarised in the principle stated below and directly links into the background of the Intent Tool in KBDS which is discussed in detail in Chapter 6.

> Issues give rise to the need to take decisions. Any difficulty in reaching a decision results in an unresolved issue. Each unresolved issue has a number of possible positions that could be adopted leading

to the generation of an increasing number of possible alternatives as the number of unresolved issues increases.

Much work has been done over the years to examine ways of dealing with uncertainty during design. Grossmann and Sargent expressed the uncertain parameters as bounded variables and undertook a design that is able to meet specification within the feasible range of the parameters whilst being optimal with respect to a weighted cost function, (Grossmann and Sargent 1978).

The generation of alternatives is some what neglected by Douglas in the rush to get an initial design, which is then subjected to improvement, down on paper. This is highlighted by the inclusion of a final level to create and evaluate alternative designs in the modified hierarchy given in (Rajagopal et al 1992 and Douglas and Stephanopolous 1994). Alternatives should be identified and noted at all stages in a design. Rudd and Watson devote the first part of their book, (Rudd and Watson 1968), to the importance of alternatives in design. They argue that all operational plants start as an ill defined statement that results from a perceived gap between the current situation and the needs of the company and / or society as a whole. To bridge the gap it is necessary to develop a specific problem statement with the difficulty being how to determine if the correct problem has been identified. Three needs are highlighted as being essential to the development of the correct problem and hence the correct solution. These are the need to be able to synthesise new situations and assess their potential, the need to be able to optimise designs and the need to be able to take uncertainty into account. Need one is addressed in Chapter 5, need two now commonly occurs through the use of simulation tools but need three is the province of alternatives generation. Rudd and Watson produced a list of questions for use in the preliminary screening of alternatives that give a very good grounding for such work. These questions are given below:

1) Is the concept illogical?

2) Can the concept be shown to be inferior to one of the alternatives suggested?

3) Can the concept be shown to be equivalent or inferior to a known inferior

processing concept?

4) Can the concept be shown to require too much technical or economic extrapolation from existing technology, thus involving too high a risk?

5) Is the concept unsafe?

6) Does the concept suggest a better alternative?

7) Does the concept involve special technical competence which is not possessed or which cannot be acquired through normal business channels?

Mansfield and Cassidy report on a framework developed to challenge the basis of a project at key steps and so promote the identification of alternatives, (Mansfield and Cassidy 1994). Additionally, the alternatives generated can be evaluated in terms of their inherent safety, cost and feasibility. Table 2 summaries this framework which concentrates heavily on the project prior to the detailed phase to ensure the greatest impact on the design. Due to the lack of reported case study work it is not possible to judge how useful the framework would be during a design.

Although it is suggested by Douglas that the first pass design could be revisited to examine possible alternatives, experience strongly suggests that, in practice, once something has appeared on paper there is a tendency to view this as "carved in stone" and difficult to alter. This can be viewed as inertia and in the same way increases as the bulk of completed work increases due to the time and money expended in reaching that point in the design. A failure to fully investigate all alternatives at an early stage in design, leading to a need to make significant changes later, leads to inefficient use of resources, an increased possibility of errors occurring, delays in schedule and higher design costs. All arise from the complications in work patterns and information flows that are a result of high levels of rework. The easiest, and cheapest, projects result when rework due to alterations are kept to a minimum and hence where the thorough investigation of alternatives and solution of issues takes place as early as possible. Phases 1 and 2 of the project structure given in Chapter 1 are the points at which this can take place most effectively as these involve the lowest numbers of people, with process engineers forming the bulk of the effort. As soon as a project reaches phase 3, front end design, the project team starts to expand and the number of disciplines involved rises.

At this point the project man-hour expenditure starts to rise steeply and the information flow becomes complex resulting in both increased costs and higher levels of difficulty when attempting to make changes. The importance of adequate investigation at the conceptual process design stage is emphasised by Berzins and Jones who point out that poor decisions taken at this stage can have a dramatic impact on the overall project feasibility, (Berzins and Jones 1989). Whilst process design is quoted as costing about 1 - 3 % of the final plant cost by the end of the conceptual design, where the bulk of this work occurs, decisions taken have fixed approximately 80 % of the plant capital cost. An interesting analogy can be drawn with playing solitaire on a computer where it is not possible to backtrack and change decisions that have lead to a blind alley. The failure rate in such a situation is much higher than when playing with cards where such "cheating" is possible. To achieve a 100% success rate without backtracking would require prior knowledge of the position of all the cards in the pack. This low cost of process work is borne out by Chambers who gives the following allocation of total project costs, (Chambers 1994), but notes that the work done in the first two phases has a major effect on the final overall cost.

Feasibility	0.1 %
Basic Engineering	0.9 %
Detailed Engineering	9.0 %
Procurement	49.0 %
Construction	38.0 %
Commissioning	3.0 %

Thus, if conceptual design is completed without allowing the optimization that arises from considering design alternatives, then it is too late to achieve serious capital cost savings. This point of view has now been widely accepted and forms the basis of a UK government initiative, ACTIVE, launched in July 1996, (Lockie 1996). ACTIVE, Achieving Competitiveness Through Innovation and Value Engineering, aims to attract process plant investment into the UK by reducing the cost of building by 30 %. The timescale envisaged for the change is three years. Five phases of a project are identified and assigned the following proportions of the total project cost:

Concept	2 %
Design	12 %
Procure	44 %
Construct	40 %
Commission	2 %

These figures are roughly in line with those from other sources. The cost reduction opportunities at the concept phase are identified as being equivalent to the -30 % target of ACTIVE. To achieve this, design must be firmed up as soon as possible and design stage problems, such as over design and late changes, be avoided. The ACTIVE initiative approach is to set up a group of interested companies under the direction of a steering group. An action plan has been developed which focuses on culture change and the implementation of good practice. As well as the impact on capital cost of process design decisions, Berzins and Johns state that they also fix 90 - 100 % of operating costs such as utility consumptions and product yields. The impact of conceptual design on plant safety is discussed in Chapter 8. These arguments can be summarised by saying that phase 1 and 2 design activities play a major role in determining the overall performance of a project and that this performance will be adversely affected by a failure to optimise by the investigation of alternatives.

4.2.2 Applicability to all Design Types

It is possible to categorise the types of process design that are undertaken using a number of different methods. A combination of the following factors is normally used to assign a "label" to any given project that provides a good indication of the extent and scope of the project.

4.2.2.1 Industry Sector.

Industries originating projects requiring process design input cover a wide range of backgrounds from Oil Exploration to Pharmaceuticals. The area of industry giving rise to the project provides a good indication of the type of materials that will be involved and hence, via a knowledge of the physical properties of the materials, the unit operations that are likely to occur. Additional factors such as likely scale

and mode of operation are also implied. For example, a Petrochemical sector project is much more likely to involve a large scale, continuous, gas/liquid plant than a Food sector project.

4.2.2.2 Mode of Operation.

Whilst this is implied by the factor above it must be clearly stated as a separate factor. In idealistic terms there are only two modes of operation, batch and continuous, but in practise batch plants have continuous elements and visa versa leading to a blurring of the distinction. This factor gives clues as to the type of equipment and control scheme that are likely to occur but can only be defined after a portion of design work has been under taken. It should be noted that a batch plant may contain equipment items which undertake more than one role in the process, whereas each item in a continuous plant will be designed and controlled to fulfil a single function.

4.2.2.3 Material Phase.

Of the three material phases that can occur, gas, liquid and solid, a plant can contain either one, a combination of two or all three. The phase or phases that are present have a great impact on the technology that is used for processing the material. This covers all aspects of plants including handling, reaction and separation. For example a crystalliser could appear on a solid/liquid plant but would not appear on a gas/liquid plant. The basic Douglas hierarchy is applicable to vapour / liquid streams only but Douglas has proposed a number of alternatives to cover both different phase combinations and all phases together, (Rossiter and Douglas 1986, Douglas 1992, Rajagopal et al 1992). Evans discusses the requirements for simulations involving solids as well as vapours and liquids, (Evans 1989). ASPEN is cited as a simulator that can handle all three phases.

4.2.2.4 Project Type.

Projects requiring process design input can range from grass roots complexes where infrastructure must be designed along with the processing units to minor modifications to operating units. This factor obviously clearly indicates the scope of work involved in a project, though within each category there is potentially a wide variation in manhour expenditure. This is particularly true for modifications that can cover anything from the replacement of a relief valve with less than a hundred design

hours to a complete revamp requiring many thousands of hours.

4.2.2.5 Design Phase.

There are a number of different schemes for defining the phases of design through which a project must pass on the way from being an abstract idea to becoming a fully functioning entity. These phases are primarily linked to the need to provide staged cost estimates in order to obtain the necessary finance and can be viewed as key hurdles in the procedure to persuade management that the project should be supported. The scheme adopted for this report has been defined in Chapter 1. This factor provides information on the amount of design work that will be involved and the deliverables that will be required. For example a conceptual design will include preliminary values of the major equipment parameters whereas detailed design will include full specification of all the required items.

A truly flexible, and useable, model of the design process, at the conceptual phase in particular, must be able to address the requirements of each feasible combination of the above factors within a single structure. Even the modified Douglas hierarchy is clearly not such a model and this in one of the major failings of the approach. However, the above specification of model requirements is a very demanding one that may well be unrealistic for a model of manageable size and complexity. Hence the question of specialisation versus generalisation comes into play and has been the subject of a great deal of debate.

Remembering that the concern here is with the early, conceptual, stages of design the final factor above can be largely ignored leading to a considerable simplification in the demands on the model. During the later phases of design the need for detailed simulation of units and streams with greatly differing structures for each category of design has lead to a proliferation of highly specialised tools. These are in addition to commonly used flowsheeting tools and cover aspects such as equipment item designs, (Kiranoudis et al. 1994), and special plant designs (Bush and Silverston 1978; Petrides et al. 1989; Elnashaie et al 1989 etc). Kiranoudis et al argues that it is necessary to provide specific simulators in order to produce accurate and robust results as the mathematical models used in many commercial simulators are simple and not suitable for detailed simulation. This view is also held by

(Eriksson et al 1990) who tested the use of ASPEN in the paper industry. Where accuracy is needed they emphasis the need for a specially designed tool. The incorporation of the ability to deal with every conceivable detailed design type into a single tool is possibly unrealistic, probably unnecessary and likely to result in an expensive tool that is a jack of all trades and master of none. However there is no reason why the model of the design process underlying the use of the tools should not be applicable in all cases.

During the conceptual phase of design the use of different models for different categories of project is to be particularly discouraged. At this stage very little is firmly known about a project and the objective is to explore alternatives whilst major changes are still possible with minimal impact on costs. The imposition of artificial barriers on the exploration task that would result from the use of a variety of methods rather than a general method would hinder this task and may result in a search that fails to come close to the optimal solution. This would provide a flawed basis for the rest of the design. It is also important to take into account the reluctance of users to apply a system that requires a multitude of methods to be learnt / relearnt each time a project of the specific type is encountered. Whilst the first reason is of a more fundamental nature for the development of models and tools to aid design, and is discussed separately below, the second will act as a natural break on the wide scale adoption of ill thought out methods and tools. Even extremely elegant solutions to design issues that are implemented in such a way as to make them difficult for the user to pick-up and use will simply not be adopted. Process engineers, and the companies that they work for, are looking for methods and tools that can be utilised without the need for a large amount of time being invested before useful results can be obtained, making complex methods that are specific to a very narrow range of problems unlikely to gain wide acceptance. Murr and Smith state that a design engineering computer aid should be straight forward to use, be able to handle changes easily, use as little data as possible and produce useful results quickly, (Murr and Smith 1996). Considering the wide range of possible project types involved in process engineering there is the possibility, particularly for contractors personnel, of considerable time gaps between the use of specific tools with the consequent need to climb the learning curve at each instance of use.

Concentrating on the artificial divides that are encouraged by an early move to separate models for different types of project this point is raised in (Gorŝek et al. 1992). They state that it is impossible to predict, at the beginning of a design, which operating mode will be able to meet the required product purity and will represent economically the best alternative. Thus forcing an early decision based on operating mode may well result in a non-optimal solution. The reliability of an early split between batch and continuous process modelling was called into question during the ADEDOPS Workshop (ADEDOPS 1995) where the debate on continuous versus discrete modelling focused on the thought that discrete models may simply be the result of sloppiness in modelling. A combined discrete / continuous simulation system, based on gPROMS (generalised PRocess Modelling System), has been developed by Unilever. Murr and Smith point to the following three reasons why a different approach must be taken to the simulation of batch processes, (Murr and Smith 1996), the scheduling problem, recycling of material between batches and the need to handle both time and state events. Von Watzdorf et al argue that dynamic modelling and simulation of batch operations is more complicated than dealing with continuous processes due to the discrete control actions imposed on the units and the logic that coordinates their operation (Von Watzdorf et al. 1994). They go on to discuss the use of gPROMS for the modelling of complex batch processes. This tool is a general purpose modelling package that can be used for both discrete and/or continuous processes which reenforces the view that it is unnecessary to adopt an approach that forces an early split between the two operating modes, as is the case with Douglas. gPROMS is an equation oriented tool that can be used for both modes. In a review paper of the state of the art, Pantelides and Barton support the view that batch and continuous processes can be modelled by the same tools, (Pantelides and Barton 1993). They point to dynamic simulation as key to addressing this.

One type of project that is consistently singled out as requiring specially adapted or dedicated modelling tools are biochemical projects. Dervakos et al point out that biological systems are generally more complex and less well defined than chemical engineering ones making it likely that traditional approaches to modelling will not be suitable, (Dervakos et al 1989). The key to this argument is that

organisms such as bacteria have complex metabolic pathways with hundreds of intermediate metabolites. Gritsis and Titchener-Hooker also discuss the differences between biochemical and chemical engineering whilst emphasising the need to develop a biochemical process simulator, (Gritsis and Titchener-Hooker 1989). The differences that are highlighted are:

(i) Biochemical processes deal with living materials that exhibit behaviour that is difficult to predict using conventional models.

(ii) Batch and semi-continuous modes of operation are used.

(iii) Unit operations that are unique to the field and can only be described by semi-empirical models occur.

Whilst there can be no argument that the first of these is unique to biochemical projects, this is also highlighted by Dervakos et al, the second and the third could also apply to many chemical processes outside the mainstream refinery and petrochemical sectors. Farza and Chéruy describe a bioprocess modelling and simulation tool, CAMBIO, developed to aid the generation of mathematical models of these processes, (Farza and Chéruy 1993). The user builds a symbolic representation of the process that is automatically translated into a mathematical model. Kinetic rates are acquired interactively and finally a dynamic simulation model is generated. In describing the use of the main stream simulator ASPEN plus for wastewater treatment process Farag and co workers demonstrate that a separate tool is not necessary for biochemical processes, (Farag et al 1990). Regardless of this point, what can be said about all three differences is that rather than being explicit reasons for special tools they could each be addressed within a general simulator containing suitable models and methods. Similar arguments are put forward as to the uniqueness of food processes, a branch of biochemical engineering. Best and co workers state that the complexity of food processes lies in the nature of the materials, their form of packaging, the equipment used and the mixture of batch and continuous processing, (Best et al 1995). However, the size of such a widely applicable simulator would exceed the capabilities of the currently available platforms. The use of an integrated environment, see Chapter 7, clears the way for the use of a collection of small tools under a unified user interface but this does not address the needs of the feasibility study and conceptual design phases. Here using

a raft of tools requires the user to make potentially restrictive judgements about the design. The current generation of commercially available simulators are generally perceived to be not good at tackling any non standard process, regardless of the originating sector, leading to the development of tools such as those described by (Fidgett and Harrison 1989) and others specific to a certain type of plant as mentioned earlier within this section. Of the tools discussed by Fidgett and Harrison, EPOS, is of particular interest as it claims to be a dynamic model capable of handling novel technology and following the project from design through to operation. This feature addresses the factor raised in 4.2.2.5. Future developments of simulation tools must address the need for wider applicability, particularly outside steady state chemical processes, if a further explosion of tools with a limited range of application is to be avoided. During the detailed design phase a balance needs to be struck between the accuracy of the model needed and the use of a wide range of tools. It should however be noted that if an integrated design environment is used, as discussed in Chapter 7, then the user is not exposed to interfaces with each of the tools used. In this situation the learning curve difficulties involved with using multiple tools are overcome and replaced with concerns over transparency and environment architecture.

4.2.3 Selection of Alternatives.

In order to be able to progress a design it is continually necessary to take decisions that effect the path of the design and hence the final outcome. These decisions range from the major, such as plant location and process route, to the minor, such as pipe diameter and the number of temperature indicators, however they all have the potential to impact on whether or not the project is viewed as a success. If sequential design with no exploration of alternatives were undertaken there would be no optimisation and a high risk of being lead up a blind alley that does not contain a valid answer to the problem. Given that the aim of all projects is to succeed it is necessary to consider both the measures of success that are relevant and how the decisions taken impact on these. The obvious statement that any project must fulfil the function for which it was designed, a bridge must stand up and a Polyethylene plant must produce Polyethylene, can be made, but other than this the success or

failure of any given project can be judged in a number of different ways, some of which will be dependant on the view point of the person making the judgement and the stage in the project life at which it is being made. In order to facilitate the choice between alternatives during the design phase it is necessary for those involved in the design to attempt to prejudge the success criterion that will be used during the operating phase. To a certain extent this involves crystal ball gazing due to the ever changing economic and legislative climate but past experience provides useful pointers.

Scott and Macleod present, based on their experience, a list of six critical process characteristics for a successful design and state a further five less quantifiable factors that will also affect the choice of process scheme (Scott and Macleod 1992). The six critical characteristics are safety, product quality, reliability, operability, predictable usages and profitability with the others being environmental impact, sensitivity to changes in commercial factors, relation to existing operations, patent / licensing considerations and previous experience of the technology involved. Peters and Timmerhaus emphasise the need to keep in mind the overall economic picture during design but state that there is a requirement to ensure that the design results in a facility that is safe and environmentally acceptable as this ultimately determines if the economic goals are met (Peters and Timmerhaus 1991). As well as safety and environmental impact, they also discuss a number of other factors, which they term general design considerations, which also impact on the ability to achieve the economic goals. These factors are plant location, plant layout, plant operation and control, utilities, structural design, storage, materials handling, patents and legal restrictions. The emphasise in Peters and Timmerhaus is, however, firmly on the need to achieve a favourable economic picture in order to receive management approval for the project. This is also the approach adopted by (Douglas 1988), which was subsequently partially modified by the inclusion of waste minimization issues into the basic hierarchy (Douglas 1992). Wells includes a chapter on what are termed "modifying considerations on costs" which are site, environmental issues, plant layout, safety, maintenance, utilities, pipework materials and sizes, control and means of operation, (Wells 1973). These factors show a marked degree of overlap with those listed by Peters and Timmerhaus and those listed in (Douglas 1988) as

"other significant aspects of the design problem" and result in projects where the design is driven by the need to optimise with respect to cost. Such an approach is backed up by a large body of literature on means of economic evaluation and cost estimation such as (IChemE and ACE 1988), (Kharbanda and Stallworthy 1988), and (Allen 1991) but it should be cautioned that not all projects can be addressed in this way. McGreavy and Han focus on a factor that they call process flexibility as being one of the principal criteria in process design, (McGreavy and Han 1989), with their usage of the term implying the robustness of the design to changes in variables and not the ability of a plant to manufacture a range of products. Given that the data used during design is always subject to uncertainty and that many market variables are outwith the control of a project, robustness is an important characteristic. Sensitivity analysis can be used to determine what magnitude of change in any given variable would result in a reversal of a decision and is used to help establish risk. This is inherent in any effective decision making process and should not require emphasis as a separate characteristic.

Returning to measures of success or failure, rather than focusing on factors that are connected with the decisions to be taken, the discussion above and experience of a range of projects suggest that the following six criterion form a good general basis for these measures. These are listed in alphabetical order to avoid an impression of priority ranking and can be viewed as responses to the question of what the characteristics of a successful design should be. The importance that is attached to each of the characteristics will vary between industry sectors and within these will vary from project to project.

(i) Clean.

(ii) Constructible.

(iii) Cost-effective.

(iv) Maintainable.

(v) Operable.

(vi) Safe.

These characteristics are discussed in the following sections.

4.2.3.1 Clean.

The environmental impact of industrial operations has come under increasing scrutiny, and legislative control, during recent history with the pace of change over the last decade being particularly rapid. During this period there has been a very significant rise in public awareness of the issue of discharges to the environment due to the activities of pressure group such as Greenpeace and Friends of the Earth. Sharratt states that UK government statistics based on a survey of public attitudes shows that the level of concern for the environment has not been diminished by the recession and remains close to the peak levels of the 1980's (Sharratt 1995). Public awareness is at such a level that consumers will make conscious decisions to avoid the products of companies that have the reputation of being polluters. This point is illustrated by the public response to the controversy surrounding the fate of the Brent Spar platform in the North Sea which involved picketing of some Shell service stations. The option of dumping in deep water that was to be exercised was subsequently abandoned and even though Greenpeace did later admit that their figures for the quantities of harmful substances contained within the structure were incorrect the whole exercise can only be viewed as a public relations disaster for the oil industry. Combined with the legislative framework which can impose significant fines on polluters, such actions make it prudent for companies to pay attention to the discharges from their operations. Even for companies that do not make the bulk of their profit by selling directly to the general public, not an uncommon situation in the chemical industry, image is important and pressure can usually be applied via investors. Concerns over public image can be clearly seen in the annual reports of companies with the trend being to include, often as a separate booklet, information on the environmental performance of the company. To avoid sending out the wrong signals care must be taken that such information is factually correct and not simply paying lip service to public concerns. It has been pointed out, (Anonymas 1995), that the environmental reports of major companies often contain misleading information and claim emission improvements that do not take into account sales of assets and plant shutdowns. Such revelations can only damage attempts to improve the public image of the chemical industry.

Since 1st April 1991 any company wishing to operate a Part A process, as

defined in the Environmental Protection Act 1990 (EPA 1990), must apply to HMIP for process authorization. Embodied in the 1990 Act is the concept of integrated pollution control, IPC, which requires companies to demonstrate that the total environmental burden of a plant with respect to land, air and water is controlled within specified guidelines in order to achieve the "best practicable environmental option", BPEO, using the "best available technique not entailing excessive cost", BATNEEC. Part B processes are regulated by local authority pollution control with respect to emissions to air and by The Water Resources Act 1991 with respect to aqueous emissions. The National Rivers Authority (NRA) takes responsibility for monitoring and taking action with respect to water pollution. Where clean-up operations are required the NRA must initially bear the costs before attempting to recover them at a later date. Reference should be made to a standard text, such as (Crittenden and Kolaczkowski 1995), for further details of the current legislative position in the UK, but it should be noted that the situation is changing almost continuously. Imminent changes are briefly mentioned below and the trend towards integration is of particular note. Under EPA 1990 HMIP have the power to demand improvements be made and can take a series of steps, ultimately leading to a prohibition notice, to ensure that these are carried out. The preparation of submissions to HMIP and complying with required improvements has placed a financial burden on the chemical industry estimated, (Ottewell 1995), to be £1.57 billion of capital, over the four year period to 1995, and £250 million/year running costs. On the positive side about £90 million/year savings are expected to result from implementing IPC due to factors such as energy savings and lower processing costs.

In April 1996 the structure of regulatory bodies within the UK changes with the introduction of Environmental Agencies, one covering Scotland and the other the rest of the UK. The new integrated organisational structure will coordinate the actions that are currently undertaken by HMIP, local authorities and the NRA and will aim to focus environmental regulation and enforcement, (Kelly 1996). The structure of the new agency for England and Wales is described by (Munns 1996) and it is emphasised that the Agency aims to be seen as an impartial regulator with public accountability. The Environment Agencies were set up as a result of the

Environmental Act 1995 passing into law with the aim of making measurable long term improvements to the quality of air, land and water. The thrust is towards sustainable development. The Act has been described, (Malcolm 1996), as the key legislative enactment of 1995. Whilst the key organisational change resulting was the establishment of the Environment Agencies the Act also deals with a number of important matters such as a regime for the control of contaminated land and the provision of powers to local authorities to designate air quality management areas. Under the Act local authorities, overseen by the Environmental Agency as necessary, are required to seek out and order the clean up of contaminated land. In contrast to the current NRA position the new act places the burden of clean up costs straight onto the original polluter or, if they cannot be traced, onto the current occupier of the land. This underlines the principle of making the polluter pay and has already started to impact on property deals with additional checks and pre-emptive clean-up projects taking place. A three month period is allowed for the responsible body to take voluntary action after which a remediation notice can be served. The forthcoming introduction of a landfill tax, at a rate of £7/Te of active waste and £2/Te for other waste, is another measure aimed at forcing industry towards clean technology which is causing ongoing projects to adopt a maximum recycle philosophy. The Act gives the Agency specific functions and responsibilities with respect to the management of water resources and aquatic environments. It has a duty to promote the conservation and enhancement of the natural beauty and amenity of inland and costal waters and associated land, to promote the conservation of flora and fauna which are dependant on an aquatic environment, and to promote the use of such waters and land for recreational purposes.

For the foreseeable future the outlook can only be towards tighter controls of emissions with both new plants requiring to be built and existing operations modified to meet the limits. Any operations that are unable to comply will ultimately be forced to close down. In addition to tighter limits there is also likely to be a trend towards banning the use and production of certain substances that are deemed to cause particularly severe damage. An example of this type of action is the phasing out of certain chlorinated refrigerants which is currently taking place within the European Union. The factors discussed above all combine to ensure that the

environmental impact of any project must be assessed now more that ever before. Traditionally waste treatment was only dealt with when the bulk of the design work had been completed, leading to a reliance on end-of-pipe schemes. This is no longer an acceptable approach to take. Manousiouthakis and Allen assert that the correct point in design to consider waste minimisation is during synthesis, (Manousiouthakis and Allen 1994). The UK adheres to the hierarchy of waste treatment options laid down in the European Community Council Resolution on Waste Policy (90/C122/02) and in the revised Framework Directive (91/156/EEC). This hierarchy starts with prevention as the preferred option and moves down through minimization and recycling to disposal, which is the least favoured option and the one that results from the use of end-of-pipe solutions (Crittenden and Kolaczkowski 1995). In order to incorporate such an approach into design, environmental impact has to be integrated into the design process. Only at the early stages of design, when the fundamental decisions on route are being made, can the opportunities for prevention and minimization be fully explored. The curve of ability to influence environmental costs against project time scale is of the same shape as that for the incorporation of safety into a design. At the initial stages there is a high ability, dropping rapidly as the project progresses. Life cycle analysis allows environmental impact for all project phases, up to decommissioning, to be considered early in the design when the ability to make fundamental changes is still high. This approach has traditionally been used in the nuclear industry. A series of five articles on minimisation in the process industry were published by Smith and Petela in 1991 / 1992. The first, (Smith and Petela 1991a), concentrated on identifying the sources of wastes, process and utility, within a process. Process waste sources were split into reactors and separation systems and means of addressing these sources covered in more detail in (Smith and Petela 1991b) and (Smith and Petela 1992a). Utility waste minimisation for unsteady state operations and utility systems were discussed in (Smith and Petela 1992b) and (Smith and Petela 1992c) respectively. A recurring theme throughout the series is the need to take an in-depth global look at systems, including developing an understanding of dynamic behaviour, in order to be able to make the fundamental changes / decisions needed to ensure minimisation.

Golonka and Brennan report on the use of life cycle assessment techniques to

carry out the comparison of environmental impact of alternative treatment scheme for emissions, containing Sulphur Dioxide, from metal smelters, (Golonka and Brennan 1996). The technique described provides a useful means of ranking alternative routes and would aid the selection of a "clean" process. An important point highlighted by this work is the criticality of the position of the system boundary used in the analysis. The ranking, by calculated environmental index, altered when downstream processes as well as the desulphurisation processes were included in the analysis.Stefanis and co workers also emphasis the criticality of the position of the process boundary, (Stefanis et al 1995). They propose a Methodology for Environmental Impact Minimization (MEIM) based on life cycle analysis. In MEIM the impact assessment is based on the emission inventory and the environmental impact of each emission. Selecting a process that minimises impact at one site to shift it elsewhere is not acceptable.

Draw backs of using life cycle analysis to select the best environmental option include the length of time needed and the quantity of detailed information necessary. During the early stages of design the technique is unlikely to be usable causing a limitation in the source reduction that can be achieved. Johnson and Flower suggest that a system of targeting be used to incorporate source reduction into the early stages of design, (Johnson and Flower 1995, Flower et al 1995). Targets for waste levels are set at a boundary around the process that includes the waste treatment facilities. The design is then steered towards these targets which could be legal limits or limits imposed by site treatment facilities. Azapagic and co workers focus on the use of multi-objective linear programming to optimise life cycle environmental objectives, technical, financial and social factors, (Azapagic et al 1996). They state that system improvements cannot be carried out on the basis of environmental life cycle assessment alone.

The background to a US initiative to develop a computer based pollution prevention process and product design system is described by (Radecki et al 1994). With strong industrial involvement from the conceptual stages the tool set described, CPAS (Clean Process Advisory System), aims to be tailored to industry's needs. At the time of writing none of the tool set proposed had been implemented. The philosophy behind CPAS is to provide the engineer with access to sufficient

knowledge on processes, techniques etc to allow informed choices on alternatives to be made. In the absence of such information it is likely that only tried and tested solutions will be considered regardless of how optimal they may be. Key to the success of such a system would be regular updates of the information included as environmental treatment options are continually expanding. Care should be taken to avoid always recommending a "new" technology when an established one may be preferable. The CPAS architecture proposed uses an integrated set of tools, each covering a specific area such as reaction pathways, regulatory advice or gas stream treatment options. Such a tool, if regularly updated, would be an extremely useful design aid.

A workshop to consider how best to incorporate environmental factors into process simulation and design tools was held jointly by the US Environmental Protection Agency, the US Department of Energy and the Centre for Waste Reduction Technology (CWRT) in 1992, (Eisenhauer and McQueen 1993). A group of invited participants from government agencies, industry and academia formed into four groups to discuss: Environmental considerations in process design, model needs, design tools and simulation and data needs. The aim was to determine fruitful areas for the concentration of research efforts. Areas identified as high priority included improved methods of synthesising chemical processes with an environmental objective, new optimisation strategies to take into account environmental factors, cost and operating requirements, improved means of costing environmental options and better methods for accessing the environmental impact of alternative process designs.

Isalski and co workers propose a HAZOP like structured approach for waste minimisation called ENVOP, ENVironmental OPtimisation, (Isalski et al 1992). ENVOP was developed jointly by contractor Costain and operator BP Chemicals and an application to a BP organic acid plant is reported. ENVOP aims to ensure that the design team looks at all the available opportunities for effluent reduction and uses cash flow analysis to rank solutions. The most cost effective solution can then be selected. Formal review meetings, based on PFD's, are proposed to firstly define the problem and apply the guide-words and secondly to review and evaluate the alternatives. In the example study reported HYSIM was used for modelling in the first phase and a Lotus spreadsheet for the economic analysis. Whilst the approach

is similar to a conventional HAZOP the guide-word set is different and the focus on PFDs not P&IDs. Bringing such an approach into a modified HAZOP system would give a great advantage in terms of minimising the number of reviews to be held and avoiding fragmentation of design factors.

Douglas has proposed an adaptation of the basic hierarchy to include waste minimisation, (Douglas 1992). Houghton and co workers build on this to examine waste minimisation opportunities in batch plants, (Houghton et al 1996). These are stated as having a greater potential, per unit product, for waste production than continuous processes. This increased potential arises from increased time spans for transient, unsteady-state operation. The adaptation proposed focuses on the inclusion of cleaning processes and the application of the method to all modes of operation. Another adaptation of the Douglas hierarchical approach to address environmental impact is described by, (Rossiter et al 1993). A seven stage hierarchy is proposed including, at Level 5, a means of looking at product drying in solids processes and, at Level 7, a means of looking at fugitive emissions from plant items. The five other levels included are as per the original Douglas hierarchy. At each level ways of minimising emissions are investigated.

4.2.3.2 Constructible.

It would appear to be an obvious statement that it must be possible to build the design but often problems are uncovered during the construction phase that require fix-it solutions to be put in place which may adversely affect the viability of the project. Frequently such problems arise due to communication failures leading to errors such as the misinterpretation of the process design intent during detailed design or violations of basic design assumptions that are not subject to rework. A typical example is that installed pipework may contain many more bends than assumed during the pump sizing calculations with the possible consequence that the purchased pump is not suitable for the required duty. If constructability is defined as doing all that is possible to make construction easy with the aim of improving quality and safety and to reduce the construction period then it is obvious that this factor can have a direct impact on project feasibility.

Fundamental constructability problems such as an inability to fit a vessel into the steelwork should rarely occur due to the use of either plant models or 3D CAD

on virtually all projects. Whilst detailed construction plans can only be drawn up during detailed design when firm information such as equipment sizes and weights, plant layout, pipe routes and the extent of civil works is available the most suitable construction methods for a plant can be agreed at a much earlier stage in the design. This early consideration of construction can be vital if delays in the project schedule are to be avoided by holding placement of civil contracts such as those for ground preparation and foundations until all the necessary information has been finalised. A multi-discipline team including mechanical and civil engineers is necessary when considering constructability but the input of process engineers is likely to be minimal. Kerridge advocates the use of multi-discipline constructibility meetings to be held from the earliest phases of design to address this issue, (Kerridge 1993). Layout issues are most likely to affect the ease and cost of construction. Process engineers have a clear input here in ensuring that material can flow through the resultant plant. This, however does not permit process engineers to proceed without regard for this issue and it should be borne in mind during the initial phases of design to avoid making unfeasible demands, for example specifying equipment of a size that is outside the normally occurring range.

4.2.3.3 Cost-effective.

This title has been deliberately chosen to avoid an implicit assumption that all design projects are profit driven. Optimisation with respect to profitability alone was traditionally used as a means of selection between alternatives with all other factors being secondary. When looking at process schemes rather than trivial choices, such as the selection of pipe sizes, profitability was judged by commonly occurring economic performance indicators such as payback time and return on investment calculated from estimates of capital and operating costs. During the early phases of design the likely profitability of alternatives is difficult to assess with any degree of certainty as accurate estimating methods require that considerable amounts of information is available and hence that an appreciable quantity of design effort has been expended. Basic information such as throughput and the number of main processing steps can be used to predict cost using costing equations prepared by the analysis of existing plant data. Davenport and Gerrard report the development of such an equation for water treatment plants, (Davenport and Gerrard 1995). For all

but commonly occurring plants such equations will not be readily available, but can be developed. Using economics as a means of selecting between design alternatives assumes that there is an adequate means of estimating the relative cost of the options being considered. During the initial phases of a design when most alternatives are being explored and ranked there is also the least information available upon which to base estimates. This is particularly a problem for novel processes where traditional methods based on existing plant cost data may not be workable. Generally, estimating methods during feasibility studies and conceptual design are based around the main plant items (MPIs) with items such as pumps and instruments allowed for by factoring. Douglas asserts that pumps can be ignored during screening but this should be used with care as if complex machines are required, eg to handle viscous fluids or raise high pressures, they can make up a significant portion of the MPI cost.

An extensive body of work exists comparing actual costs to estimated costs in order to refine the methods but there must always be a question mark over their accuracy. If two options have estimated economic performances that are close it would be foolish to discontinue pursuing one on this basis. Tools such as ICARUS, (Smithson 1995), have been developed to apply expert systems to cost estimation, the aim being to aid decision making and selection of alternatives. ICARUS utilises a knowledge base containing rules of thumb, objects and procedures. Simulation results, with additional data if a high level of detail is required, are used to obtain the equipment information needed for the costing. This provides an estimating tool that could be used by the process engineer as soon as simulation runs are commenced. This moves the engineer away from a reliance on published cost charts where the basis may not be clear. In the authors experience of such charts they tend to produce reasonable results for vessels, but give under estimates for exchangers, pumps and compressors. This may distort the selection of alternatives. They are also not easy to use for non-standard items where previous data is not available in sufficiently large quantities for anything other than a sparse chart.

When there is a high degree of uncertainty in the parameters used in a design then it is not possible to prepare a single definitive economic case but only to define the likely envelope of economic performance. The robustness of the design to

changes in parameters is important as if the degree of sensitivity to change is high then the risk of moving into the economically unfeasible region is high. Parameters to be considered can be those involved in the design or those related to the external economic climate in which the project must perform. There is a direct relationship, based on the level of uncertainty, between the cost of preparing an estimate, covering the design work necessary to provide the data as well as the manipulation of numbers, and the accuracy of the value obtained. Initial estimates prepared for a project will often only be to an accuracy of ± 50 % and even these require sufficient multi-discipline design effort to make them too expensive to be prepared for a large number of design alternatives. Consequently, fundamental decisions about the structure of the process are often taken by the process engineers without the preparation of an estimate, although very rough economic comparisons can be used. These decisions fix a high level of the project cost with a commonly quoted figure being that 5 to 10 % of the design effort fixes approximately 85 % of the total cost.

Given the continually tightening legislative framework with respect to health, safety and the environment, discussed separately, it is no longer acceptable to make design choices purely on the basis of profitability. Karlström and co workers point out that designing to objectives such as flexibility may cause conflict with profitability as increased capital costs will be incurred, (Karlström et al 1992). Some projects, such as those that occur to deal with wastes generated from existing plants, will never be profitable but they should be cost-effective. To be cost-effective the design intent should be attained and the legislative requirements complied with for the best possible combination of capital and operating cost. Traditional techniques for investment evaluation such as return on investment and payback time do not easily allow for the inclusion of factors like environmental impact that cannot easily be expressed in monetary terms. Pickering suggests that assigning risks to each of the costs and cash flows allows a better picture of the environmental aspects associated with an investment to be developed (Pickering 1995). The technique results in an expected monetary value (EMV).

4.2.3.4 Maintainable.

To a certain extent it could be argued that the ability to maintain a plant is directly linked to the ability to operate it as a plant that cannot be maintained will

cease to operate as break downs occur. However as the method of approach to maintainability and operability during design are significantly different the two characteristics should be discussed separately. A maintainable plant is one that can be kept in a state suitable for operation providing that certain routines are carried out on a regular basis. The percentage of the time that the plant is physically able to perform is referred to as the availability or occupacity, which is a function of the time between failure or shutdown, the reliability, and the time needed to return the plant to operation after such events, (Lamb 1996). Whilst Lamb refers to the latter factor as maintainability this implies a much narrower focus to the term than is meant here where it is used to cover the whole range of concept inherent in high availability plants. Undertaking maintenance on a plant costs money due to the manhours that have to be expended, the cost of spares and consumables and any associated down time with consequent reductions in availability. If maintainability can only be achieved by an extensive maintenance programme to overcome reliability problems the economic viability of the plant may well be compromised. To avoid such a situation it is not sufficient to simply buy and slot together a series of hardware items that are known to possess sufficiently good reliability characteristics to minimise the items maintenance requirements. As each item does not act in isolation without interference, the system containing it and the mode of operation adopted must be considered when attempting an overall minimisation of maintenance costs whilst ensuring that the plant is sufficiently reliable to meet occupacity goals. The techniques of reliability-centred maintenance (RCM), (Jones 1995), have been developed using this approach and takes place during plant design using a multi-disciplined team including process engineers. Using failure data analyzed to identify the root cause of the failure, the technique allows maintenance plans to be drawn up and also helps establish areas where there is a reliability risk. Alternative approaches to RCM are maintenance-centred and availability-centred techniques. The first of these is the oldest of the three and focuses on the maintenance cycle to improve the efficiency of the cycle. Reliability improvements, if they occur at all, are coincidental rather than an integral part of the technique. The availability-centred approach is introduced by (Lamb 1996) who claims that it represents a new way of doing business. Both maintenance and reliability are to be engineered and managed

using a four phase plan in order to ensure a competitive advantage. These four phases are as follows:

Phase I - How the plant fits into the overall company structure is determined and measures of performance identified.

Phase II - An understanding of the current plant performance against the factors identified in phase I is developed.

Phase III - A model of plant availability performance is developed and tested.

Phase IV - The model is used to identify pressure points that can be used to improve performance and implementation issues are addressed.

No practical examples of the use of the availability-centred technique are discussed making comparison with the more established techniques difficult.

A strongly mathematical approach to addressing maintainability during design is presented by (Thomaidis and Pistikopoulos 1994). Here a superstructure model of the system is built using data on the process, equipment reliability and costs. This MILP problem is then solved to give the optimal maintenance strategy. The quantity of data required is unlikely to be available during the early stages of design, when equipment has not been selected, casting doubt on the practicality of this approach.

It is unrealistic to expect mechanical devices to run without periodic attention and very few people would consider treating a car in such a way as even if missing services may save money in the short term the risk of major, expensive failings that could have been prevented if treated sufficiently early is too high. Common to all mechanical devices there is a need to undertake regular preventative maintenance, such as topping up oil levels and cleaning filters, and less frequent planned overhauls. Unfortunately due to the costs involved in carrying out such a programme there is a tendency, when money is tight, to take a short term view and resort to running on break down maintenance only. Under this regime only things that go wrong are fixed, although statutory inspections obviously still take place. Whilst this may seem attractive initially when reliability and availability are high long periods operating in this mode will reduce both factors as items start to fail due to neglect. Even given an adequate maintenance programme reliability will fall steeply if any items are not fit for purpose. This failing can arise for a number of reasons with

some of the most common being:

(i) Incorrect specification of materials of construction leading to high levels of corrosion / erosion and ultimately loss of containment.

(ii) Poor quality of manufacture resulting in mechanical failure.

(iii) Inability of the purchased equipment to meet the specified duty.

(iv) Errors in specifying the required duty leading to the purchase of equipment that cannot fulfil the in-service duty.

These factors can be split into two distinct groups, those arising from the reliability of the equipment and those arising from a failure to correctly specify the required duty. The reliability group may be outside the control of process engineers and subject to decisions taken by the purchasing department unless adequate reasons for rejecting a bid can be found during evaluation. Suitable reasons are knowledge of poor previous performance and a lack of vendor experience of the technology involved. Unless there is good reason to explore the use of unproven technology or to believe that the lowest priced items will be technically suitable then the best option in the long term is often to ensure the purchased items are robust even if this involves paying a premium. The failure to correctly specify the required duty is almost exclusively within the control of the process engineer as the production of specifications is one of their major roles during design. Attention to detail and adequate checking are necessary during design to minimise the likelihood of specification errors occurring. Some items such as bulk steelwork and many control system elements fall outside the scope of process engineering and here the responsibility lies with the relevant discipline engineer.

An additional factor in the maintainability of a plant is the requirement to ensure that maintenance can actually be carried out. Particularly important are the needs to ensure that adequate access and means of isolation are provided. At a simple level access could be provided by the installation of a platform to allow an item that needs checking regularly to be reached but more complex measures such as the need to provide sufficient access for cranes and heavy machinery to carry out less frequent tasks such as pulling the tube bundle of an exchanger may also be necessary. Generally access issues are layout related and are addressed during

detailed design via the use of layout drawings, a scale model of the plant or 3D-CAD. The provision of isolation, via valving arrangements of varying complexity, can be tackled earlier in the design during the production of P&IDs and should be covered during a HAZOP study.

4.2.3.5 Operable.

Whereas maintainability is related to the mechanical running of individual items of plant equipment operability concerns the ability of the plant to function as a single entity producing the desired outlet streams. Alternative names for this characteristic could be controllability or flexibility but the first of these tends to be associated solely with the performance of control systems and the second with the reaction of the process to disturbances that enter it. Morari defines controllability as the ability of the system to accomplish the dynamic transition between operating states in an acceptable manner and flexibility as the ability of the system to handle a new situation at steady state, (Morari 1992). An alternative definition of flexibility is applied to plants, generally batch, that are capable of producing a range of different products. Both alternative names fail to address the broader implications of operability. For a plant to be operable not only must the control system be capable of maintaining parameters within the required range, the goal being stable operation without the need for continual operator intervention, but the plant elements must be correctly specified for the duty within this range. Stable operation gives the benefit of low variability in product quality with the associated benefits of saleability and customer satisfaction. No control system can overcome gross mismatches between design and specified duty such as the presence of an additional phase or large differences in throughputs and conversely a plant made up of well designed items of equipment will not function correctly if the manipulated and measured variables are incorrectly chosen. As plants become more highly integrated, for environmental and economic reasons, the issue of operability will become increasingly important. To be adequately incorporated it must be considered from the earliest stages of design. The HAZOP process, discussed in Chapter 8, is designed to address operability as well as hazard identification, hence the name, but the "OP" section generally tends to be less well addressed. To make the best use of

the technique this shortcoming needs to be addressed.

The correct specification of plant items and the design of the control system necessary for stable and safe operation cannot be completely divorced from each other, hence the need to address operability from the earliest stages of the design process. This issue has been addressed by a number of workers including (Fisher and Douglas 1985, Bekkers and Rijnsdorp 1992, Karlström et al 1992, Huang and Fan 1992). Herman and co workers propose a coupling of SpeedUp and the process control system ACS to form SPEEDWACS in order to integrate process design and control, (Herman et al 1985). SPEEDWACS was envisaged as being a tool of use in process design, dynamic simulation, operator training and control strategy development. Etzkorn and Arkun propose an equation oriented simulation tool, CHESOPS, making use of user interaction and graphical output to couple process and control design, (Etzkorn and Arkun 1980). CHESOPS went part of the way to becoming a dynamic simulator. Using a simulator as a basis implies a tool that can only be used after the synthesis stage of design has been completed. To address operability adequately it must be included from the earliest phases.

The first workshop of the International Federation of Automatic Control (IFAC), held in 1992, was convened to address the perceptions that difficult process control problems often resulted from poor plant design and that better design would result if control issues were addressed early in a project. The plenary address at the workshop consisted of a review of work in this area, (Morari 1992). Morari concentrated on controllability evaluation and split the work into three categories: steady-state, linear dynamic and non linear dynamic models. Bouwens and Kösters discuss an industrial case study of control system design where it was found that completely different optimal solutions were found when equipment and control system design were integrated as opposed to the latter following the former, (Bouwens and Kösters 1992). Fisher and Douglas point out that if equipment is designed for a set of operating conditions chosen in a rather arbitrary way without regard for operability then the resultant plant may well be vulnerable to small disturbances in the variables. To address this a hierarchical procedure for assessing steady-state operability is proposed. This only tackles part of the requirement for operability as the ability to control unsteady-state operations such as start-up and

shut-down are also important. Long and difficult start-ups can have a significant impact on plant performance by eroding the period for which the design intent is being met. Bekkers and Rijnsdorp describe a tool called EPIC (Early Process design Integrated with Control) which is aimed at involving control engineers in the early stages of process design. The aim of EPIC is to evaluate controllability and assist in the choice of the most suitable control structure. Further details of EPIC are provided by (Rijnsdorp and Bekkers 1992). As alternative flowsheets are generated by the process engineers they are assessed for stability and controllability by the process control engineer. This aids selection of alternatives with the most promising flowsheets being analyzed in more detail to determine the behaviour under various modes of operation as well as considering the economic performance. The main element of the EPIC user interface is the Process Instrumentation Matrix (PIM) table which aids the selection of the controlled and manipulated variables. The algorithm for stability evaluation within EPIC is based on Bode's minimum phase criterion. Laing and Ponton propose a methodology for concurrent process and operating system design that uses a similar approach to EPIC, (Laing and Ponton 1992). The hierarchical model of design is used as a basis for integrating the two aspects of design and co-ordinating the efforts of the process engineer and the process control engineer. Laing and Ponton term the latter role "operations engineer". The hierarchy for the control system is based on operating nodes of which there are three general classes: Regulatory nodes maintain a process at a stationary state, transition modes move from one stationary state to another and executive nodes select the appropriate node based on the process state and constraints. Operating nodes are analogous with the plant sections, reaction, separation etc, used in the process design hierarchy. The design of an operating node is developed as a design progresses with precision, robustness and parsimony being the main design objectives. At a high level in the hierarchy only large scale, in terms of magnitude and time scale, disturbances can be considered due to the low level of design information available. As this detail is added other disturbances can be considered. Laing and Ponton point to conflicts between the aims of the two aspects of design as being a factor that requires special consideration. The same workers have also proposed a simpler hierarchical approach, following the Douglas methodology, for control system

design, (Ponton and Laing 1993). Here the thrust is towards aiding the process engineer place control loops appropriately. Barton and co workers also propose a hierarchical method based on the Douglas methodology and discuss case study work, (Barton et al 1992). Another worker adopting an approach based on Douglas is Padley, who modified the basic five level hierarchy and performed synthesis using both versions to indicate the impact of considering operability early in the synthesis, (Padley 1991). The more highly heat integrated flowscheme produced by the basic procedure was rejected on controllability grounds when the problem was analyzed by the modified version. Padley found that it may be helpful, from an operability point of view, to delay the decision on batch / continuous operation, see earlier discussions. Levels 1 and 2 of Douglas remained almost unaltered but for an increased emphasis on gathering data on disturbances. At levels 3, 4 and 5 operability is addressed after the basic process synthesis has been completed. After classification of disturbances into fast and slow flexibility and controllability are considered separately. Flexibility is addressed by optimising the design within the upper and lower bounds of disturbances, with design rework as necessary to ensure feasible operation. Controllability is addressed by looking at open-loop stability, the choice of controlled variables, right-half-plane zeros and sensitivity to modelling errors. An alternative approach is proposed by Luyben and Floudas who incorporate controllability measures into the MINLP problem for design, (Luyben and Floudas 1992). This work is further expanded by (Luyben and Floudas 1993). The aim of Luyben and Floudas was to develop a systematic procedure for addressing controllability issues from the earliest stages of design before a flowsheet had been produced. They also consider heat integration. A multi-objective problem involving economic, control and heat integration objectives has thus to be solved. They propose a four step procedure to achieve this. Firstly a superstructure containing all the possible design alternatives of interest is constructed. This is transferred into an MINLP model including mathematical expressions of the constraints. The MINLP is then solved to generate the non-inferior solution set from which the best compromise solution is extracted by an algorithmic method. Huang and Fan adopt a similar approach and propose a distributed strategy that takes into account the criterion for controllability simultaneously with those for process design at the

synthesis stage, (Huang and Fan 1992). They define controllability as the ability to perform under transient conditions and the ability to reject disturbances when in a given operating mode. The lack of information at the synthesis stage caused difficulties during the development of the strategy which were resolved by the used of a quantitative knowledge based approach. Concepts such as degree of intensity of disturbance and level of control precision were represented as mathematical equations and heuristic knowledge as production rules. Controllability is assessed by examining the vectors of inlet disturbances and outlet control level and the matrix of disturbance propagation. Examples based on HEN and MEN problems are presented by Huang and Fan.

During the design of any plant and the associated control system the operating companies preferred method of plant operation must be taken into account. Whilst the norm is for automatic control and the subsequent reduction in necessary manning levels this may not be the case for plants located in regions of the world where labour is cheap but parts for a sophisticated control system are expensive and difficult to obtain. The need to use a level of technology appropriate to the application is a requirement that should be applied to all aspects of design.

4.2.3.6 Safe.

Most plants within the process industry contain materials that constitute a hazard to the health of any person that becomes exposed to them or to the consequences of their hazardous properties. The following list of hazards associated with the process industry is based on (Coulson et al. 1983).

(i) Flammability. Given the correct combination of concentration, oxygen level and energy source a flammable material will burn. The particular set of conditions applicable to a given combustion reaction determine the ferocity, which can be explosive.

(ii) Explosions. An explosion is a sudden, catastrophic, release of energy that results in a pressure wave. Whilst explosions are often associated with the burning of flammable materials they can occur in the absence of fire due to the release of pressure energy from the rupture of pressure containing equipment such as air receivers.

(iii) Toxicity. Almost all materials are poisonous to some extent with the

level of hazard depending on the toxicity and both the frequency and duration of exposure. Some materials cause immediate injury even at low levels whilst the effects of others may only become apparent after long periods of exposure. In addition to poisoning deaths due to asphyxiation, commonly in nitrogen environments, are also a hazard. Reference should be made to COSHH Regulations 1988 (HSC 1988) for the legislative aspects of exposure to hazardous substances.

(iv) Pressure. Each element of a plant will be designed to withstand pressures within a specified range and there may be an associated risk of abnormal conditions causing either over or under pressure leading to the risk of loss of containment. Catastrophic over pressure leads to the risk of an explosion, see above.

(v) Temperature. As with pressure each element of a plant will be designed to withstand a given temperature range. Moving outside this range can lead to loss of containment due to drastic reductions in the strength of materials of construction. Even within the operating range extremes of temperature pose a risk if it is possible for people to come into contact with the containing surfaces and receive burns, hot or cold.

(vi) Noise. The most common source of noise on a plant are the drives and motors associated with the provision of motive force. Other possible sources are the flaring of materials, burners and releases of high pressure steam. Exposure to high levels of noise causes hearing damage and noisy plants can expect to have poor relationships with the surrounding community.

(vii) Corrosion. Whilst generally not itself a hazard corrosion can, if undetected or rapid, lead to loss of containment.

An important point to note is that hazards in each category should not be viewed in isolation as worst case scenarios often occur due to a combination of events that, if they occurred singly would not constitute a major risk. For any plant there exists an envelope of conditions that define the limit of safe operation outside which the likelihood of an incident rises rapidly due to the existence of hazardous situations. This envelope is different to that which defines the plant operating limits.

Due to the number of parameters involved in a design the bounds of the envelope cannot be defined by point values of single parameters. Dimitriadis and co-workers define the space of potentially unsafe conditions as a union of hyperrectangles in the state variable space, (Dimitriadis et al 1995). This means that they are defined as combinations of ranges of values for the various process parameters. Regardless of the properties of materials it can be argued, (Burgoyne 1986), that all accidents are ultimately caused by some form of human failing. This could be in design, construction, operation or management. The area of human factors in safety will not be expanded further here. For a safe plant it could therefore be argued that all human elements should be removed from a plant. As this is not possible it is therefore necessary to concentrate on ways of reducing or containing the hazards.

In addition to this list of hazards the process industry is also prone to more general hazards present in all manufacturing operations. These general hazards cover such aspects as the dangers from falling from heights, being struck by falling objects, tripping over objects, contact with rotating equipment and electrocution. It is virtually impossible to design all hazards out of a plant, particularly the last group as people will always have accidents, but it is the duty of a designer to ensure that the plant that is built represents as small a risk as possible both to those working on it and those living in the vicinity. It also represents a good business strategy as replacing damaged plant is expensive both in terms of capital cost and lost production. Additionally, as with environmental issues, companies with a poor safety record are likely to have a correspondingly poor public image which will last a considerable time after an incident, with the extent of notoriety being linked to the number of fatalities. In the minds of the general public the name of Union Carbide will be linked to Bhopal for many years as will Occidental be linked with Piper Alpha. The moral duty of care for those who could be effected by the operation of a business is backed up by legal requirements as expressed by the Health and Safety at Work Act 1974 (UK Government 1974), the various amendments and supplements to this act, and the UK implementation of the European Community Seveso Directive (82/501/EEC) and the Control of Industrial Major Accident Hazards (CIMAH) Regulations, 1984, with subsequent amendments. The implementation of the Seveso Directive saw the advent of the preparation of safety cases. The directive is not a

static tool but is constantly under review by a panel of experts drawn from member states. Prior to the 1974 Act the main legislative tools were the various Factories Acts and the Chemical Works Regulations policed by the Factory Inspectorate. The legislative framework within the UK is aimed at achieving health and safety at work through self-regulation. To achieve this the acts of parliament, such as the Health and Safety Act state broad principles and enable secondary legislation, Regulations, to address specific areas. Detailed guidance is given in documents such as Codes of Practise which represent the best current practise. This set up allows a flexible legal framework that can react quickly to advances in technology. Self-regulation will only prove to be effective if industry resists the temptation to submit to economic and scheduling pressures when dealing with health and safety issues.

As indicated by the name of the EC directive much of the driving force for the initial legislation came from major accidents that occurred in the 1970's, notably Flixborough (1974) and Seveso (1976), and unfortunately this trend of reactive legislation has continued. The impact of the Flixborough accident, in the same year as the HSE was formed, on the approach to design safety in the UK can be judged by considering the recommendations of the Advisory Committee on Major Hazards (ACMH) set up in the wake of the explosion. One of the main problems faced by this committee was defining what criterion should be used to categorise a plant as a major hazard, (Schenkel 1976). The three pronged strategy towards the control of major hazards proposed consisted of identification, prevention / control and mitigation, (Williams 1992). A legislative programme to implement the strategy commenced with the introduction of the Notification of Installations Handling Hazardous Substances Regulations in 1982 and continued until the European Community became active in this field. The quantity of published work also rose sharply. Early work in this field was presented at sessions of the IChemE symposium series entitled Chemical Process Hazards with Special Reference to Plant Design. This series began in 1960 and still continues under the revised series title of Hazards, (IChemE 1960, 1963, 1967, 1972 and 1977). Subsequent work has resulted in an extensive body of literature covering this topic. Examples are (Wells et al. 1976), (Kletz 1984) and (Scott and Crawley 1992) with chapters on this subject appearing in all modern design texts such as (Coulson et al. 1983) and (Peters and

Timmerhaus 1991). In an address to the Hazards IX conference in 1986 Millar of the USA Environmental Policy Institute highlighted Flixborough and the lack of an equivalent accident within the USA as being the prime reason for US legislation on major hazards lagging behind that in the UK, (Millar 1986).

The Flixborough and Seveso accidents were of a very different nature. The first being a vapour cloud explosion, Cyclohexane, resulting in 28 fatalities and wide spread damage and the second the release of a toxin, 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD), leading to no human fatalities but long term land contamination and wild life fatalities. That both accidents, one an immediate catastrophe and the other a more insidious threat of long term damage, have had such a major impact raises the important question of what constitutes a major hazard. Wilson proposes a system for comparing the threat of different materials based on the concept of a common "damage zone" beyond which the effects of an incident are tolerable, (Wilson 1980). To give a quantitative measure of comparison the amount of material which, if released under standard conditions, would produce a "damage zone" covering an area of one square kilometre is put forward. For toxic material the damage zone is that one square kilometre rendered uninhabitable for one year, for materials with more immediate effect fatality figures can be used. The results reported were close to the, then draft, UK regulations on the quantities of materials that define a notifiable hazardous installation.

In order for a project to be judged a success the variables associated with determining the characteristics discussed above must be considered from the earliest stages of the design process. The best approach would seem to be a modified HAZOP technique requiring a systematic examination of a design from the earliest phases, with all the factors considered simultaneously. The importance weighting attached to each characteristic will vary from project to project. It would be a pointless exercise to expend the time and effort, and hence incur the cost, in designing a plant that had, for example, unacceptable emissions even if the resultant design was optimal with respect to, for example, cost. This point is emphasised by (Mansfield and Cassidy 1994) who concentrate on safety but state that it must be integrated with other factors such as economics, technology and time at all stages of

a project. Similarly Azapagic and co workers concentrate on environmental impact but state that technical, financial and social factors must also be considered to achieve system improvements, (Azapagic et al 1996). Stephanopoulos highlights economics as the predominant factor considered during optimization but mentions that other considerations should also be included, (Stephanopoulos 1980). Factors mentioned are operability, controllability, safety and reliability. All the targets must be considered concurrently if the design is to approach optimisation with respect to more than one or two of them. The Douglas hierarchy fails to address all these points but they will be addressed in the alternative hierarchy proposed. The basic Douglas hierarchy has been modified to take into account some of these factors, (Douglas 1992), but treats them as add-ons not integral with the design. They must be fully integrated at all stages. The move towards integrated design environments, see Chapter 7, shows a trend towards such an approach.

4.2.4 Use of Design Heuristics

To make a rapid progression between the levels of the hierarchy Douglas makes extensive use of design heuristics, also referred to as rules of thumb and design guidelines. These are simple expressions that summarise the previously gained experience of solving design problems of the type to which the heuristic applies. Historically heuristics would have been developed over a number of years by those actively undertaking "real" designs but today they are more likely to be the result of a researcher running a large number of case studies and then attempting to identify a pattern in the results. This approach makes it easier to identify the limitations of the heuristics. Typical of the examples quoted by (Douglas 1988) are the following:

> "Whenever a light reactant and either a light feed impurity or a light by-product boil lower than propylene (-55 °F, -48 °C), use a gas recycle and purge stream."
>
> "It is desirable to recover more than 99 % of all valuable materials (we normally use a 99.5 % recovery as a first guess)." etc.

As Douglas points out virtually every heuristic has some limitations, with

particular problems resulting from the assumptions used whilst formulating the heuristic. There is an inherent danger in applying heuristics developed by others that, unless the full background of development is known, the use may fall outside the range of applicability and thus negate the use of the heuristic. This danger is amplified if inexperienced users attempt to use apparently simple heuristics drawn from books without attempting to investigate the limitations. There is a tendency, even amongst those who should know better, to latch onto anything that solves a pressing problem and not to take the time to question the method being used as long as an answer is produced that addresses the immediate requirement. Amongst those with more experience there is an equally worrying inclination to develop a set of "pet" heuristics that are applied in all cases without any real thought. Another problem with heuristics is that conflicts can arise between them. Methods of dealing with contradictions are therefore needed.

In order to avoid re-inventing the wheel with every design that is undertaken and to act as aides-mémoire some form of prior knowledge capture and encapsulation is necessary. Design heuristics are a popular means of achieving this as can be seen from their regular occurrence in standard texts such as (Coulson et al. 1983), (Perry et al. 1984) and (Peters and Timmerhaus 1991) and also from the existence of a number of books devoted to them, for example (Fisher 1991) and (Ganić and Hicks 1991). These latter books cover a wide range of disciplines and tend to be devoted to only commonly occurring rules rather than design heuristics specifically applicable to plant design. The use of heuristics in plant synthesis is discussed in Chapter 5.

4.2.5 Inclusion of Heat Integration

At level 5 in both the original and modified hierarchical models due to Douglas energy integration is considered. This is late in the design process after the bulk of the process has been synthesised. The method used to incorporate heat integration is the well known method of pinch technology as developed by Linnhoff and co-workers, (Linnhoff and Flower 1978). This work has become generally accepted and whilst the original concept remains unaltered, additions now allow the technique to be applied to a range of situations. Developments allow areas such as emissions targeting, batch process integration and retrofitting projects. As pointed

out by (Schembecker et al 1994) the design of heat exchanger networks using this method is primarily a tool for analysing a flowsheet and not for synthesising it. Therefore to conform to this limitation it is correct, if pinch technology is used, to only consider heat integration after synthesis has been completed. Such an approach rests on the assumption that good, close to optimal, solutions to the design problem can be generated by ignoring heat integration until the basic flowsheet has been selected. This assumption has been challenged by a number of workers, (Aggarwal and Floudas 1992), (Linnhoff et al 1990), (Dhallu and Johns 1988), (Kakhu and Flower 1988), (Lang et al 1988), (Muraki and Hayakawa 1987) and (Nishida et al 1981), who claim that it is necessary to consider heat integration during synthesis to obtain an optimal solution. If a sequential approach is adopted and process conditions such as operating pressures are optimised before heat integration is applied the resultant flow scheme could be less economic than that resulting from a simultaneous approach. Lower utility costs in the latter case can shift the optimal point towards a higher conversion factor and hence reduced raw material costs, (Lang et al 1988).

Stair and Fraga show that ignoring heat integration during the initial stages of synthesis can lead to a misleading ranking of solutions, (Stair and Fraga 1995). If a designer selects the designs to pursue further on this basis it could lead to an optimal solution being discounted. However, the simultaneous consideration of separation sequence and heat exchanger network, for example, considerably increases the complexity of the problem. One possible method for simultaneous consideration is to develop a superstructure containing the possible sequences to be considered which is then solved by MILP. No heat exchange structure is included but minimum utility consumptions for an assumed minimum temperature difference are included in the optimisation. This becomes cumbersome as the number of alternatives rises. Linnhoff and co workers introduce a method based on Pinch Technology that claims to give greater insight into the problem, (Linnhoff et al 1990). Grand composite curves are used to identify the effects of changes in utility selection, process modifications and capital/energy optimisation on each other. This forms the basis of the suggested procedure. An alternative approach is proposed by Sandoval and Zhu who attempt to reduce the problem complexity of a simultaneous approach by

adopting a three phase hierarchy to the synthesis of distillation sequences and the associated HENs, (Sandoval and Zhu 1996). The problem is decomposed into separation sequence screening, HEN synthesis and HEN optimisation.

4.3 Application to a Case Study

Rather than re-visit the design of the HDA process, which has been extensively reported, the manufacture of Methyl Ethyl Ketone (MEK) was selected as a case study for the application of the Douglas hierarchy. The main reason for working with this process, rather than the HF Acid used as a test case elsewhere, was the quantity of published information available, (Austin and Jeffreys 1979). This was also the case for the work on the CHiPS package described in Chapter 5.

Austin and Jeffreys identify three methods for the manufacture of MEK:

(i) Synthesis from refinery gas.

(ii) Dehydrogenation from 2-Butanol.

(iii) Selective oxidation of 2-Butanol.

The dehydrogenation reaction is stated as being the most economical and is used as the basis for the design detail contained within the book. For synthesis from first principles it would be necessary to examine the reasoning behind this statement and consider all the alternative paths until the most satisfactory in terms of the factors described in Section 4.2.3 had been selected. However in this case, due to time limitations, only the pre-selected route will be examined.

4.3.1 Basic Reaction Information.

One molecule of 2-Butanol is dehydrogenated to give one molecule each of MEK and Hydrogen in accordance with the following equation:

$$C_4H_{10}O \dashrightarrow C_4H_8O + H_2$$

This is a gas phase equilibrium reaction which is endothermic, with a heat of reaction of 73900 kJ/kmol at a temperature of 450 °C. A Brass catalyst is used. Reaction temperature is subject to the following constraints:

(i) The rate of formation of MEK is negligible below 300 °C.

(ii) Cracking of 2-Butanol increases sharply above 400 °C.

(iii) The upper temperature limit for the catalyst is 500 °C.

The equilibrium constant is given by:

$$\log_{10}K_i = (2790/T_i) + 1.510 \log_{10}T_i + 1.871$$

The rate equation is:

$$r_c = \frac{C_i[p_{Ai}-(p_{Ki}p_{Hi}/K_i)]}{p_{Ki}[1+K_{Ai}p_{Ai}+K_{AKi}(p_{Ai}/p_{Ki})]}$$

Where:

$$\log C_i = -(5964/T_i) + 8.464$$

$$\log K_{Ai} = -(3422/T_i) + 5.326$$

$$\log K_{AKi} = (269.2/T_i) - 0.1959$$

Increasing pressure drives the equilibrium in the direction of the reactant and is therefore undesirable.

4.3.2 Initial Conclusions.

Based on the reaction information and a small amount of additional information it is possible draw some preliminary conclusions about the likely reaction process and to propose a basic block flow diagram, this is shown in Figure 1.

From the reaction information it can be said:

(i) It will be necessary to pre-heat the feed, whatever the phase, to the reactor to achieve the necessary reaction temperature.

(ii) To maintain the reaction temperature, given that the reaction is endothermic, it may be necessary to heat the reactor.

(iii) At the outlet of the reactor it will be necessary to separate the unreacted 2-Butanol, for recycle the MEK product stream, and the Hydrogen, a possible fuel stream.

Given the additional information that the 2-Butanol feed and the MEK product will be in the liquid phase whilst the reaction is gas phase it is possible to add:

(iv) The reactor fresh feed and recycle streams will require vaporisation.

(v) The hot reactor discharge gases will require condensing.

(vi) There is the potential for heat integration between the reactor feed and discharge streams.

Basic knowledge of the physical properties of the compounds involved allows the following to be stated:

(vii) Condensing and phase separation will result in a liquid stream containing MEK and 2-Butanol and a vapour stream of hydrogen saturated with MEK and 2-Butanol.

(viii) MEK and 2-Butanol can be separated by distillation.

(ix) The organic vapours contained within the Hydrogen stream should be considered as candidates for recovery with a possible approach being absorption followed by separation. Using water as the absorbent indicates the need for a solvent extraction due to the presence of azeotropes.

4.3.3 Level 1, Batch versus Continuous.

Level 1 is used by Douglas to gather background information needed to undertake the design and to take the decision between batch and continuous operation. Three factors are considered as a basis for this decision.

(i) Capacity. The required production rate given by Austin and Jeffreys for the MEK plant is 1 x 10^7 kg/year (2.2 x 10^7 lb/year). This is above the limit of 10 x 10^6 lb/year given by Douglas as being normally continuous.

(ii) Flexibility. The MEK plant has only a single product that is not subject to seasonal demand nor expected to have a short life span. All these point towards the use of a continuous process.

(iii) Operational problems. Excessive fouling is not expected. Slurries are not handled. The reaction is not slow. All these point towards continuous operation.

Level 1 decision : Continuous Process

No safety, economic or other considerations have gone into making this decision. Safety could be incorporated if factors such as inventories of hazardous materials and the probability of cross-contamination were included. The use of economics to support the decision on mode of operation would not be possible until later in the design when capital cost estimates for the two options become available. Environmental impact also requires more design work for sensible consideration but

it could be noted at this stage that the variable composition of waste streams from batch plants often makes them difficult to handle. Constructibility, maintainability and operability would be difficult to incorporate meaningfully very early in design. It is highly questionable if it is necessary, or desirable, to make the decision on operating mode at such an early stage in the design without any ability to look at the optimality of the choice.

4.3.4 Level 2, Input - Output Structure of the Flowsheet.

With the route preselected in this case study, and by Douglas, valuable opportunities for including inherent SHE aspects, in addition to economics, in route selection by considering alternatives are missed. The failure to adequately acknowledge and track alternatives is one of the key shortcomings of the Douglas method. Manually handling a number of alternatives could be difficult but tools such as KBDS, see Chapter 6, could make this much easier. Only a single route will be considered from now on.

At the simplest level the MEK process can be represented, as shown in Figure 2, as a black box with 2-Butanol entering and MEK and Hydrogen leaving. Using this as the basis for running through the decisions that Douglas takes at Level 2.

4.3.4.1 Purification of Feeds. There is only one feed to the process as shown, 2-Butanol. Although it is known that there will be additional feeds into the separation area these cannot be derived from the diagram as shown. No information on possible impurity levels in 2-Butanol is included by Austin and Jeffreys, who assume the feed alcohol is pure. Industrial chemicals virtually always contain impurities which can, even at ppm inlet levels, eventually build-up to concentrations where problems result in a plant not designed to handle them. However without a full laboratory analysis of the feedstock, addressing this issue is not possible. As such an analysis is often dependant on plant location it is unlikely to be available during the early phases of design. This decision would have to be re-evaluated as and when more information becomes available.

Level 2, Decision 1 : Feed purification facilities are not applicable.

4.3.4.2 Recovery or Recycle of Reversible By-products. This is not applicable in this case as there is only a single reaction known for the scheme under consideration.

4.3.4.3 Gas Recycle and Purge. The reaction takes place in the gaseous phase but

to remove the product Hydrogen from the reactor exit is likely to take place using condensation. Thus the recycle of unreacted 2-Butanol will be liquid, the boiling point exceeds the -48 °C given by Douglas for light components to be considered for gas phase recycle, so there will be no gas phase recycle.

Level 2, Decision 2 : There will be no gas phase recycle and purge.

4.3.4.4 Limited Recovery and Recycle of some Reactants. The decision whether or not to recycle some of the unreacted feeds exiting the reactor must be based on the economic balance of separation costs against increased raw material costs and on a consideration of the ultimate destination of the material that is not recycled. In this case, any 2-Butanol not recovered for recycle is assumed to be burnt. The economic data used as a basis, extracted from a number of sources, is as follows:

Selling price of MEK = £25.45 / 100 kg

Cost of 2-Butanol = £7.77 / 100 kg

Value of Fuel stream = £1.01 / 10^6 kJ

Value of Hydrogen = £1.57 / kmol

The cost of the 2-Butanol is sufficiently high to make it a candidate for recovery and recycle. Without cost data it is not possible to determine a sensible target for the fraction recovered. Safety and environmental impact are not factors.

Level 2, Decision 3 : 2-Butanol should be recovered and recycled.

4.3.4.5 Number of Product Streams. The main product will be MEK. Unreacted 2-Butanol will be recovered and recycled as far as practical. Hydrogen may be used as a fuel stream containing hydrocarbon vapours or be purified leading to separate Hydrogen and fuel streams.

Level 2, Decision 4 : There will be 2 or 3 outlet streams and one recycle.

4.3.4.6 Economic Trade-off of Variables. Initially assuming 100% conversion with 1 mole 2-Butanol giving 1 mole MEK and 1 mole hydrogen.

Required MEK = 1 x 10^7 kg/year = 138,889 kmol/year

2-Butanol required = 10,277,778 kg/year

Hydrogen produced = 277,778 kg/year

Raw material cost = £798,583 per annum

Product revenue = £2,545,000 per annum

Hydrogen revenue = £218,056 per annum

Economic potential = £1,964,473 per annum

This assumes that Hydrogen and hydrocarbons are separated with the Hydrogen used for catalyst regeneration rather than use it as fuel. However this type of decision cannot be taken until equipment costs can be added into the picture.

If the conversion is dropped to 90%, the value indicated as achievable by Austin and Jeffreys, the economic potential falls to £1,917,448 per annum if it is assumed that the separated alcohol is used as fuel, Figure 3. This is still sufficiently good to make it worthwhile moving forward with the design.

Level 2, Decision 5 : Economic potential is high enough for the design to continue.

4.3.4.7 Level 2 Conclusions. Given the detail in the block flow diagram shown in Figure 1 as opposed to that shown in Figure 3 a question mark is raised over the advisability of ploughing through the Level 2 process if it is possible to derive a greater level of detail without it. The ability for multiple entry points into a design methodology is required to accommodate varying degrees of prior knowledge.

There is a very large jump between the factors being addressed in levels 1 and 2 of the Douglas approach, hinging on the level of information on the reaction system, feed quality etc assumed to be available at the conceptual design stage. In my experience of conceptual design, meaning the design of new processes with no prior history, the chemistry is still being defined long after the initial flowscheme has been developed. An indication of the gap is given if it is considered that Austin and Jeffreys' work, which goes much more into detailed engineering functions such as equipment design, does not contain all the information needed to complete the Level 2 decisions. A reason for the high level of information assumed could be that the Douglas text is a development of an undergraduate course which would utilise example processes where there is a high level of background information available.

At this stage in the design development it is difficult to take informed economic decisions due to the absence of equipment costings to balance against losses of material. Whilst, as at Level 1, constructability, maintainability and operability cannot be addressed meaningfully at this level of detail, environmental impact and safety considerations should be brought into play when recycle / waste stream

decisions are to be made.

4.3.5 Level 3, Recycle Structure of the Flowsheet.

At level 3 Douglas aims to add detail to the reactor system but leave the separation system, with the exception of any gas recycle facilities required, as a black box. This aim raises the question of whether it is possible to achieve an optimal design, even at the very early phases of design, if the reaction and separation systems are decoupled, particularly if there are recycle streams involved. The selection of reaction parameters determines the reactor outlet composition and hence the separations that are necessary but this is not a one way process. For example, if the conditions selected produce a stream that requires difficult or expensive separations the selection made must be reconsidered to determine if these unit operations could be avoided. A model of the design process must take into account the need for interplay between the various plant areas.

Running through the decisions listed by Douglas for this level.

4.3.5.1 Number of Reactor Systems. This is a single reaction step process with no need to move away from a single reactor stage.

Level 3, Decision 1 : One reactor stage.

4.3.5.2 Number of Recycle Streams. Given the presence of only a single reaction step with a single feed there will only be a single recycle stream, 2-Butanol. The reactor exit stream will be gas which, if sticking to the Douglas scheme of not considering the separation system at this stage, indicates the need for a gas recycle with some form of pressure raiser. However, as condensing is the most sensible way of separating the Hydrogen and hydrocarbons, the recycle can be assumed to be liquid.

Level 3, Decision 2 : The only recycle will be liquid phase 2-Butanol.

4.3.5.3 Excess Reactants. Given the reaction stoichiometry involved this is not applicable in this case.

4.3.5.4 Heat Effects and Equilibrium Limitations. The reaction is endothermic therefore adiabatic operation is not possible and it will be necessary to supply heat to the reactor. Even though this is not done by Douglas it was found to be necessary to examine the effect of varying temperature on the reaction system at this point. Austin and Jeffreys contains data on the variation of conversion with temperature

which shows that to achieve high conversions it is necessary to run at as high a temperature as possible. The temperature limitations given in Section 4.3.1 apply and indicate that to avoid significant cracking an upper temperature limit of 400°C should be chosen. In the absence of further information on the cracking reaction no losses to cracking were assumed below 400°C, thus setting the upper limit at this temperature. The lower temperature limit was set at 320°C, the temperature that gives the 90% conversion quoted by Austin and Jeffreys. The means of maintaining the reactor at the elevated temperatures discussed needs to be considered at this point. Heat transfer into a gas phase reaction taking place over a solid catalyst is not particularly easy but can be achieved by careful reactor design. Austin and Jeffreys adopt a packed tube reactor. It was therefore assumed that the reactor feed be heated to 400°C and that the exit temperature be 320°C. At the average temperature of 360°C the conversion is 94% and the reactor heat load 346.65 kW. Using the heuristics contained within Douglas direct heating to achieve the transfer required will be used.

Level 3 , Decision 3 : The reactor will be heated directly.

4.3.5.5 Shifting of the Equilibrium. To shift the reaction in favour of the product would require the removal of hydrogen from the reaction system. Given the short residence times within a gas phase reactor this is not feasible.

4.3.5.6 Effect of Reactor Costs. Douglas reproduces the rules on selecting a reactor type given in Levenspiel, these are not really of much use for the reaction system under consideration. The use of a plug flow tubular reactor will be assumed. Without undertaking more reactor design work it is not possible to put a cost to the reactor but, due to the type and the conditions, an excessively expensive piece of equipment is not expected.

4.3.5.7 Level 3 Conclusions. The desirability of separate consideration of the reaction / recycle section and the separation section is questionable unless the opportunity for an extensive amount of interchange exists.

In may respects Level 3 appears to be much less complex than Level 2, it is certainly less confusing. Other than a brief mention of economics none of the six criterion for success mentioned earlier in the chapter are mentioned. As reactor conditions are discussed it is expected that safety should be mentioned to allow, if

possible, inherently safe reactors to be chosen. Additionally the possibility of environmental impact for low conversions or the presence of side reactions should be considered.

The flowscheme at the outlet of Level 3 is given in Figure 4.

4.3.6 Level 4, General structure of the Separation System.

Level 4 considers the structure of the separation system by firstly considering the phase of the reactor outlet stream, termed the "reactor effluent" stream by Douglas. In this case the reactor outlet stream is all vapour. The heuristic of cooling to 100°F (37.8°C) to attempt a phase split is then applied as this is said to be the cheapest form of separation. This limit is dictated by the cooling water temperature and would therefore be location dependant. Considering the boiling points of the components in the reactor outlet stream:

Hydrogen : Non-condensible under achievable conditions.

MEK : Boiling point = 79.6°C

2-Butanol : Boiling point = 99.5°C

Condensing using cooling water and a subsequent phase split would therefore not be a problem without the need to move to a pressurised reactor or the use of a refrigeration loop. The structure of the separation system will thus be as shown in Figure 5, a condenser followed by a phase splitter with separate liquid and vapour systems. Douglas refers to the vapour system as recovery which rather prejudges the form of the process and will not be applicable in this case. The more general term of vapour separation system is preferred. Considering the vapour and liquid systems in turn.

4.3.6.1 Vapour Separation System. As this process does not have a vapour recycle stream much of the discussion included by Douglas does not apply. In this case the main choice for this system is whether to include a means of recovering the hydrocarbons carried over with the hydrogen or to accept their loss in the gas stream. If no attempt is made at recovery there will be an economic penalty associated with the loss of both feed and product materials and the ultimate destination of the hydrocarbons may well have an environmental impact. Including facilities to accomplish the recovery will require capital and entail running costs. As a first step

towards making this decision it is necessary to consider how much hydrocarbon will be lost with the hydrogen. This could be done using heuristics but is just as easy to carry out using a simulation tool. Here the problem, defined as shown below was run in ASPEN.

Problem Definition: Condenser outlet temperature = 35°C
Condenser outlet pressure = 21.95 psia
Phase separation carried out at atmospheric pressure
Reactor outlet temperature = 320°C
Reactor outlet pressure = 29.2 psia
Outlet stream composition taken from Figure 4, without adjustment for recovered material.

It should be noted, for detailed equipment design, that the high level of non-condensibles in the reactor outlet stream will result in low heat transfer rates and the need for a large exchanger surface area. With the above specification the flashed vapour and liquid stream compositions are as shown below in Table 3.

Table 3 - Preliminary flash mass balance.

Component	Vapour kg/hr	Vapour kmol/hr	Liquid kg/hr	Liquid kmol/hr
Hydrogen	34.9879	17.3561	0.0073	0.0036
MEK	262.3398	3.6382	989.4204	13.7215
2-Butanol	6.6864	0.0902	75.6446	1.0205

The economic potential for the process drops by 18% to £1,572,740 pa. On this, rather crude, analysis it would appear to be desirable to have hydrocarbon recovery facilities. Therefore these will be included at this stage. Five vapour separation techniques are listed by Douglas for consideration, Condensation, Absorption, Adsorption, Membrane Separation and Reaction Systems. Absorption or Adsorption are possibilities if suitable agents can be found. Austin and Jeffreys use absorption into water, cheap and safe, but finish with the use of trichloroethene as a solvent to separate the hydrocarbon and water. This would no longer be environmentally acceptable. Because of possible problems with the selection of

suitable materials the option of using refrigeration to condense at a lower temperature was investigated. The freezing points of the hydrocarbons are as follows:

MEK = -85.9°C

2-Butanol = -114.7°C

Initial results obtained by modifying the previous ASPEN run to cool the whole of the reactor outlet stream to temperatures below those that can be achieved by cooling water alone indicated sufficiently significant reductions in hydrocarbon losses achievable by this approach to justify a more detailed consideration. For example by dropping to -10°C losses of hydrocarbon are reduced 13 fold. To avoid the high cost associated with chilling the whole reactor outlet stream a two stage condensing system should be considered. With this system the cooling water condenser remains, followed by phase separation and chilling of the vapour stream to recover more hydrocarbon. Modelling this system using ASPEN indicated that to match the composition given by Austin and Jeffreys for the Hydrogen stream post treatment would require chilling to -30°C, this Hydrogen stream specification would require confirmation at a later stage. The cost of the refrigeration plant being balanced against a number of factors:

No solvent or solvent handling facilities required.

No absorbent or absorbent handling facilities required.

No Absorption column.

No Extraction column.

These changes represent a significant drop in plant capital and operating costs. There are only a limited number of heat transfer medium that can be used at low temperatures. Ethylene Glycol solutions can be used to -27°C but below this proprietary transfer medium or brines are necessary. Each medium has disadvantages in terms of cost, hazardous properties or corrosive properties. Selecting a compromise outlet temperature of -25°C allows a range of possible refrigerants to be carried forward to detailed design. Figure 6 shows the flowscheme resulting from the first part of Level 4 and the associated mass balance is given in Table 4.

4.3.6.2 Liquid Separation System. The function of the liquid separation system is, essentially, to separate the MEK product from 2-Butanol, for recycle. The low levels of Hydrogen carried forward from the two phase separations will be assumed to be

carried out of the process in the MEK stream at this stage. A note for the detailed design phase would be for the inclusion of some form of non-condensible removal facilities at a high point in the system. The Douglas heuristic that distillation becomes expensive if the relative volatilities of the liquids are less than 1:1 indicates that distillation is a feasible option for MEK and 2-Butanol where the ratio is 2.1:1. No azeotropic problems are anticipated therefore distillation will be selected as the separation technology, with only a single column necessary . MEK is the lighter of the two components and will therefore be recovered as the column top product. As the column feed streams are the product of condensing stages, with an approximate temperature after mixing of 28°C, it can be assumed that column preheating will be required. Figure 7 shows the flowscheme revised to show the liquid separation system. Taking the specification given by Austin and Jeffreys as a basis for a preliminary column design for completion of the mass balance.

Top product = 99.0 wt% MEK

Bottom product = 99.0 wt% 2-Butanol

The resultant balance does not quite balance but is sufficiently accurate at this stage.

4.3.6.3 Level 4 Conclusions. Very little mention is made by Douglas of any of the criteria of success at Level 4, although the inclusion of economic factors is inherent in some of the heuristics used. The inclusion of environmental impact when looking at factors that effect the plant outlet composition is essential. At this stage, where the selection of equipment has commenced, some discussion of operability and maintainability issues should be included. It is still probably too early to include constructability. At a very basic level it is not necessary to carry out much equipment design to reach the end of Level 4 and obtain a starting point flowscheme, this is the aim of Douglas who considers the screening of alternatives and optimization separately. For the reasons stated early this is not judged to be an acceptable approach, with integration of such activities into all stages of the design seen to be the way forward.

4.3.7 Level 5, Heat Integration. Options for heat integration appear to exist between the reactor feed and product streams and between the column feed and reboiler streams. These possibilities were not pursued further during the case study.

Controllability issues must be included when looking at the possibility of exchanging equipment inlet and outlet streams against each other.

4.4 The Proposed Model of the Design Process

To summarise the objections to the model of process design proposed by Douglas in a number of guises:

1) The generation of alternatives is not adequately addressed. This should be an integral part of the process, considered at each stage. During the initial phases of design a great many alternatives will be generated and only those with obvious flaws, economic, safety etc, can be discounted. Short comings in data availability will prevent a choice being made between the others. Due to time and financial constraints it is possible that some alternatives will be parked for attention at a later date. Such activities should be clearly recorded.

2) Different forms of the model are proposed for different design types. To be effective, particularly during the initial phases of design, a model should apply to, preferably, all, but at least a wide range of design types. This should cut across industry sectors, modes of operation, material phase, project type and design phase. Comments added to the questionnaire reinforce this point.

3) Success factors other than economics are not integrated into the model. To ensure that the chances of project success are maximised all six criterion for success must be addressed within the design process model to ensure that the resultant plant is clean, constructible, cost effective, maintainable, operable and safe. Question 2.5 of the questionnaire covered this point and the responses received indicated that this is an area that causes wide spread concern.

4) Reliance on design heuristics. Whilst heuristics are important in order to ensure that designs are not grid-locked initially they should be used with caution unless their background and range of applicability is clearly understood.

5) Late inclusion of heat integration. As heat integration can have a significant effect on the viability of alternatives it has to be included from the early phases of design.

It is necessary to determine how the shortcomings of the Douglas method can be addressed. Table 1 gives the seven step model proposed for this purpose, this was presented in (Marsh and Ponton 1996). The approach suggested by (Mansfield and Cassidy 1994) addresses some of these concerns particularly in the area of generation and selection of alternatives. One of the main points addressed is the inherently iterative nature of design. Recycle between levels during a pass through a model and repeated runs through all the levels with increasing amounts of detail are necessary to achieve this. The levels of the proposed model are discussed in turn below. By including a description of the input information required at each level it is possible to judge which level is most appropriate as an entry point for each project, not all will pass through all seven stages. This model concentrates on the first two stages of the design process, feasibility studies and conceptual design, but could be readily extended to cover the later phases.

4.4.1 Level A, Main Route Alternatives.

Objective: To identify all the possible process routes that can result in the desired product or consume the available raw materials, depending on the starting point for design.

To achieve this the input information required is simply a basic statement of the objectives and requirements and a clear understanding of the business objectives that are applicable. Whilst a literature survey for information on existing alternatives may be sufficient, new routes provided by R&D efforts may also need to be included. In the latter case the time scale required is extended to allow proof of concept work to be carried out to underpin the proposed flowscheme or schemes. Preliminary screening of alternatives generated at this stage is based on economics, safety and environmental impact. Economic screening at this level is based on the difference between the price of products and the cost of raw materials, with an assumed conversion based on the best information available. Safety screening is achieved by undertaking the first stage of the hierarchical HAZOP procedure

described in Chapter 8, with the alternatives ranked on the basis of the outcome. Environmental screening considers the materials involved with each alternative in terms of their hazardous properties and ranks the alternatives based on the combined threat of all the materials. At all times during the screening the basic project objectives should be borne in mind.

End product: An economically screened list of alternatives, with safety and environmental rankings, to carry forward for further development.

4.4.2 Level B, Definition of Reaction System.

Objective: To produce a complete set of reaction equation and design data associated with these equations.

For systems that do not involve reaction stages this level is omitted.

To achieve the objective, as complete list as possible of components, including impurities, in the feed streams is required. It is highly likely that there will be a need to recycle to this level as feed specifications reach a higher level of refinement and the existence of recycle streams is defined. As well as identifying all the equations of the reactions between the components present, data on these reactions must be gathered from published sources or determined by experimentation. The information required is on stoichiometry, kinetics, conversions, heats of reactions and the effect of varying reaction conditions. For systems with a catalyst activity, selectivity and life become important. The completeness of the list of components present will directly impact on the quality of the output from this stage. The economic, safety and environmental screening carried out during Level A can be refined at this stage. Economic screening can be refined by considering the quantity of feed lost to by-products over the likely range of operating conditions. If applicable, preliminary catalyst costs can be included. Safety and environmental screening must be revisited to assess the impact of any additional compounds involved in by-product reactions. Combinations of conditions that result in reactions outside a safe operating envelope should be noted at this stage, for example temperatures at which thermal decomposition occurs and the occurrence of exothermic reactions that could run away.

End product: A fully defined set of reaction equations for each option with limits on safe operating conditions. Economic, safety and environmental rankings

adjusted as appropriate.

4.4.3 Level C, Processing Stages.

Objective: To determine, without undertaking detailed design, which of the five basic processing stages will be necessary. These five stages, Feed Treatment, Reaction, Separation, Feedstock Recycle and Waste Treatment, form the basis of all process plants. Utility systems form the sixth stage and are assumed to be necessary for all processes.

The required input information is a full, or as near as possible, definition of the feed streams and reactions occurring and physical property information on the components present including an indication of potential problems, such as azeotrope formation, that could require special treatment. At this level the work undertaken will be split into the ten stages outlined below, and will be focused above equipment design.

i) If reactions are present the process will require a Reaction stage. If not go to stage vi.

ii) Examine the reaction data to determine the likely envelope of reaction conditions and hence the product spread. Aiming for high conversion and / or completion may not lead to an optimal plant overall and there will need to be a recycle to this stage once the impact of reaction stage output on the downstream plant is understood. However in order for the design to move forward it is necessary to take a judgement on the likely best way forward.

iii) From the physical property data determine the phase or phases of the components present within the envelope defined in stage ii.

iv) Identifying differences in phase between the feeds and the compounds in the reaction envelope indicates the need for Feed Treatment and for the provision of a heat or cold source.

v) Further factors that will determine the need to include a Feed Treatment stage are:

a) The removal of catalyst poisons.

b) The removal of compounds that react to consume valuable raw materials.

c) The removal of any compound that does not react but is more

difficult to remove from the product than from the feed.

vi) Unless there is only one product that will meet the required specification without treatment a Separation stage will be necessary.

vii) Identifying differences in phase between compounds in the reaction envelope and products indicates the need for a phase change as part of the separation process and for the provision of a hot or cold source.

viii) The presence of significant quantities of valuable reactants at the outlet of the reaction stage, due to factors such as low conversion, indicates the need for Feedstock Recycle. What is significant can be judged by determining the economic impact of loss of the feedstock on plant economics, assigning fuel value to the material lost. It is unlikely that it will be economically sensible to recycle materials that have an intrinsically low value.

ix) The presence of recycle streams, unless these leave the Separation stage pure, requires the Reaction stage to be revisited to consider the impact of impurities. Purging to remove such substances may be necessary.

x) The presence of compounds other than the desired product / products in the Reaction stage outlet which cannot be recycled or used as by-products indicates the need for waste streams. These will, unless they are completely innocuous, require Waste Treatment.

As additional materials are not introduced at this level and conditions remain within the bounds established during Level B the environmental ranking of the options will remain unaltered. Safety should be reassessed by carrying out the second stage of the hazard study procedure described in Chapter 8. Economic rankings may be altered by operations such as the removal of impurities from the feedstock and the recycle of unreacted feedstock and will have to be revisited.

End Product: For each alternative still under consideration a refined block flow diagram showing the processing stages required. The reasons for including each step should be clearly noted as this forms part of the design history. At this level the initial identification of recycle streams has been included.

4.4.4 Level D, Production Definition.

Objective: To produce a set of alternative process flowschemes for the front

end of the plant including Feed Treatment, Reaction and part of Feedstock Recycle.

The input information required for this stage is a block flow diagram of each alternative showing the processing stages needed, definition of the reaction system, physical property data and knowledge of the alternative technologies available. The definition of the reaction system behaviour may include assumptions that need to be tested. The work to be undertaken can be split into the five stages outlined below, those steps associated with reaction systems can be omitted as necessary:

i) Establish a best guess of the likely reaction conditions, with due consideration of safety and conversion issues. At this level the emphasis should not be placed on optimisation except for the simplest single stage reactions which rapidly achieve completion. Attempting to optimise reactor conditions without considering impact on the separation system is not a meaningful exercise. Given the likely reaction conditions the associated product spread and heat of reaction can be determined.

ii) For the conditions chosen determine if the reaction / reactions will be homogeneous or heterogeneous, remembering to take into account the presence of any necessary catalysts. For heterogeneous reactions mass and heat transfer effects have to be taken into account during design.

iii) Determine the feasible reactor types for carrying out the reaction. For homogeneous reactions consider batch, plug flow and mixed flow reactors, bearing in mind the need for mixing and / or heat transfer. For heterogeneous take into account the differences in flow behaviour of the different phases and the need to move material between phases to achieve inter-phase contact, e.g. bubbling gas into liquid, passing gas over a stationary solid phase, fluidised beds etc. Both batch and continuous reactors should be considered. Given the heat of reaction determined during Level B the need for heat transfer into or out of the reacting mass has to be taken into account.

iv) Using the feed temperature and pressure dictated by the reaction conditions and any need to remove materials from the feed identified at Level C, the equipment necessary to treat the feed can be determined. Pumps or compressors may be necessary to raise pressure, let down stations to lower pressure, heat exchangers or furnaces to raise temperature and heat exchangers to lower temperature. The

removal of undesirable materials requires the use of one or more of the available mass transfer unit operations, distillation, membrane separation, liquid/liquid extraction, adsorption etc. The appropriate treatment method depends on the phase to be treated and the physical properties of the materials.

v) If the need to recycle feedstock was identified during Level 3 the need to provide pumps or compressors to reintroduce the material into the reactor has to be considered. These are likely to be necessary as the pressure driving force through a plant starts at the reactor and runs down through the separation train, to minimise the number of pressure raisers needed.

At this level it is possible to start considering factors other than economics, safety and environmental impact when looking at the selection of alternatives. Operability can be brought into the picture by considering if the alternatives under consideration could be operated in a safe manner, e.g. if the reaction is exothermic can the temperature be controlled in such a way that the a run away reaction is avoided. The introduction of new materials at this stage should be limited, but if refrigeration is required the environmental and safety impact must be considered along with the cost impact. Ranking of the alternatives in terms of economics may be affected by the requirement for additional plant items in some cases.

End Product: Alternative flowschemes.

4.4.5 Level E, Treatment Definition.

Objective: To produce a set of alternative process flowschemes for the back end of the plant including Separation, Waste Treatment and, part of, Feedstock Recycle.

The input information required for this level is similar to that required for Level D, and for plants including a reaction system Level D should have been completed before attempting Level E. There should be a block flow diagram of the process showing the Processing stages required, physical property data and knowledge of the alternative technologies available. The completion of Level D will define the reactor product composition and conditions. As there is a strong possibility that there will be recycle streams between levels D and E it could be argued that these should be combined into a single level. Splitting the two and

allowing iteration breaks the design into manageable chunks. The work to be undertaken at this level can be split into seven stages:

i) For each of the reactor outlet streams determine the number of streams that will leave the separations stage by assigning components to recycle, product, by-product and waste destinations. Initially separations are assumed to achieve perfect splits.

ii) Look for phase mismatches between streams leaving the process, product, by-product and waste, and the reactor outlet. This indicates that the separation stage will need to include the appropriate phase changing equipment. Commonly this will involve a gas phase outlet that must be condensed to give a liquid product.

iii) For multiphase reactor outlet streams or processes requiring more than one phase of outlet stream consider the requirement for phase splitting as the first step of the separation sequence. This may follow a phase changing step. The products of the phase split are then fed to the appropriate separation processes.

iv) Treatment methods to be considered for vapour streams are: Condensing processes (high pressure or low temperature), Absorption, Adsorption, Membrane separations and Reacting systems. For gas recycle the need for a compressor will have been identified during Level D but there is a need to consider stream temperature and the use of a purge, to avoid the build-up of inerts or other undesirable materials. Valuable material will also be lost with the purge and will affect process economics. For gas product streams the design must ensure that the sale specification is met. If additional streams are introduced to achieve the separations they must undergo the same safety, economic and environmental impact assessment as the materials previously considered.

v) For the separation of liquid streams distillation is, in general, the least expensive way of separating liquid streams and should be used as the starting point for design. Potentially difficult separations due to close physical properties or the presence of azeotropes will require an alternative separation method. Consideration should be given to Liquid / liquid extraction, Extractive distillation, Azeotropic distillation, Reactive distillation or Crystallization. Column sequencing to achieve the necessary separation can follow a number of general rules: Remove corrosive components first, Remove reactive components first, Products and recycles as

distillates, Most plentiful first, Lightest first, High recovery last, Difficult separations last and Favour equi-molar splits. Pumping requirements for liquid recycle streams will have been identified at Level D but there is a need to ensure the streams have a suitable composition and the correct temperature. For liquid product streams the design must ensure that the sale specification is met. If additional streams are introduced to achieve the separations they must undergo the same safety, economic and environmental impact assessment as the materials previously considered.

vi) If solids are present simple physical separations such as filtration or settlement may be sufficient. The need to purify the solid phase will lead to more complex schemes such as selective dissolution and recrystallisation. For solid product streams the design must ensure that the sale specification is met. If additional streams are introduced to achieve the separations they must undergo the same safety, economic and environmental impact assessment as the materials previously considered.

vii) The applicable emission limits for all waste streams should be established. If at all possible consideration should be given to changes in the process that remove the waste stream or at least minimise it. Any waste treatment and disposal systems included will have a negative impact on the economics of the process. Consider processes such as neutralisation for relatively innocuous liquid streams, scrubbing for gas streams, cyclones to remove dust, incineration for all types of waste etc.

For the process to be operable the plant must produce products and by-products to an acceptable specification and have waste streams within the permitted limits. Additionally operability can be addressed by considering if the separation sequence proposed could be successfully started up, run and shut down. If it is not possible to produce a viable separation scheme without entailing excessive costs it will be necessary to recycle to Level C to determine if altering reaction conditions could allow this to occur. If not, the design may have to be abandoned at this point. Environmental and safety rankings must be revisited at this stage in light of any additional materials introduced. Flags can be raised on the economic rankings based on the number of main plant items involved but no estimating can be carried out until

sizing has taken place.

End Product: Process flowscheme for the complete plant for all alternatives. Reassessment of safety and environmental impact.

4.4.6 Level F, Basic Process Design.

Objective: To develop the design to such an extent that preliminary mass and heat balances have been produced. These should contain preliminary optimisation achieved via sensitivity analysis.

The input information at this level consists of a process flowscheme, physical property data and some means of modelling the unit operations involved. The use of a computer based simulation tool makes sensitivity analysis easier by allowing many values of the variables to be examined relatively easily. Development of the design at this level could proceed without such tools but due to their wide availability it is assumed that they would be available to the designer. The work undertaken at this level can be split into four stages:

i) Consider if the plant will be batch, continuous or a mixture of the two. Factors to bear in mind are plant capacity, number of products, demand pattern, fouling and reaction time. Large throughput plants are more likely to be continuous. Batch plants provide greater product flexibility and can reduce lead time to market. Products with a strong seasonal demand tend to be produced in batch plants that only operate for part of the year. If fouling rates are sufficiently high to require frequent shut down for cleaning a batch plant should be considered. Long reaction times may lead to a batch reactor in order to limit equipment size. The use of batch unit operations may permit some of the major items identified during Levels D and E to be combined as several unit operations can be carried out in a single piece of equipment.

ii) Set up a model of the plant using the available simulation tool. The initial set up should include the best guess values of the design variables but the permitted range should also be noted.

iii) The model using the best guess variables should be run to give a base case against which preliminary optimization and heat integration can be carried out. Neither of these can be fully exploited at this level. The effect of varying the design variables within the permitted ranges can then be examined by undertaking multiple

runs. Heat integration opportunities can be established by considering the large heating and cooling duties. If these are significant the plant may not be economic unless integration is carried out. As layout has not yet been considered pumps can only be included in standard positions or where large pressure differences are known to exist. This is not meant to indicate that pumps are considered to be unimportant.

iv) Preliminary equipment sizing can be undertaken using the balance information produced. The sizing should be of sufficient detail to allow a cost estimate to be produced.

With an estimate based on the sizing of equipment the economic ranking of alternatives can be further refined. The availability of sizing also allows maintainability and constructability to be considered for the first time. Level G undertakes this screening.

End Product: Preliminary design with heat and mass balance and equipment sizes. Some account taken of optimisation and heat integration.

4.4.7 Level G, Screening.

Objective: To identify those alternatives that are worthwhile carrying on to the next stage of the design process. Undertaking additional design to help make this decision will cost money and should be avoided.

The input information required is equipment sizes and a heat and mass balance. Screening based on all six criterion for success should be carried out at this level. Safety can be addressed by carrying out the third stage of the hierarchical hazard study procedure described in Chapter 8, this also includes operability issues. Environmental impact should be addressed by considering the fate of all materials in the process during normal operation and upset conditions. Preparing a cost estimate based on the equipment sizes allows return on investment figures to be assigned to act as an economic screen. Maintainability and constructability can be addressed by taking into account previous experience. Separate rankings against all six factors should be prepared and used to determine the way forward. The recommendation on whether to pursue a design or not depends on the judgement taken on what is acceptable, the target will be set by those outside the design team. Spending more time and money at this level would allow more confidence in the basis of the

recommendations but may not be acceptable. Equally well it may not be acceptable to carry too many designs forward to the next stage, where design costs increase rapidly.

End Product: A recommendation of a limited number of, preferably one, flowschemes to be subjected to the next level of design.

4.5 Case Study

The proposed model has been applied to the preliminary design of a HF Acid plant. In an academic environment the absence of business drivers and difficulty in obtaining data make it difficult to make such case studies realistic, but a pass though all the stages gives an idea of the functionality. Due to the similarity between the options to avoid repetition only Option 1 will be progressed beyond Level C.

4.5.1 Level A.

The production of HF Acid is an established industrial process for which there exists a large body of published information, including a number of patents. In order to manufacture HF a source of F^- and a source of H^+ are required. The most commonly used source of F^- is the naturally occurring rock Fluorspar which contains CaF_2. Another possible raw material is SiF_4, a by-product from the manufacture of fertiliser from Phosphate rock, but this has the disadvantage of being a difficult compound from which to extract the Fluoride. Additionally, the economic viability of this process is dependent on the ready availability of raw material from more than fertiliser plant. Other than opportunistic builds where feedstock is available, the SiF_4 route can be discounted. This case study will be based on using Fluorspar as the source of F^-. The H^+ can come from any acid that is available in the necessary quantities, with the acid anion forming a salt with the calcium when the HF forms. Sulphuric acid is commonly used as it is both readily available and results in the formation of $CaSO_4$, which as gypsum has a limited market for the manufacture of plaster board and related products. This case study will be based on the use of Sulphuric acid as the source of H^+. There are a number of different ways in which the acid can be fed into the system:

i) Concentrated acid (93 to 99 %). The water associated with weaker acid causes problems with the flow of material within the system and with the

concentration of product HF, see Level E.

ii) Oleum. This form of the acid can be used to further reduce the quantity of water within the system.

iii) Mixture of concentrated acid, SO_3 and Water. Feeding part of the acid requirement as Sulphur Trioxide and Water vapour allows the exothermic reaction between these materials to provide some of the heat of reaction for the main reaction.

The three alternative schemes are shown in Figure 8. As the only difference between all three is the form of Sulphuric acid used the only screening that can be done is on this basis. The results of the stage 1 hazard study are discussed separately in Chapter 8. Economically Option 1, using the concentrated acid is cheapest, followed by Option 3, using mixed feed, and Option 2, using Oleum. In terms of the environmental impact many of the substances being handled are unpleasant but Oleum causes the greatest concern. The environmental and safety rankings concur with the economic ranking.

4.5.2 Level B.

As a first step towards defining the reaction system it is necessary to define the components that will be present in the feeds. With the exception of mineral Fluorspar all of the materials to be used will be assumed to be pure. Even though acid grade Fluorspar is pre-treated, by floatation, it is a naturally occurring material and there will be variations in composition. Some traces of the chemicals used during the floatation may be present but these will be discounted at this level. A typical composition will be taken to be as follows:

	wt %
CaF_2	97.00
$CaCO_3$	1.50
SiO_2	1.00
Sulphur	0.03
Water	0.47

The main reaction equation is:

$$CaF_2 + H_2SO_4 \text{---} > 2HF + CaSO_4 \qquad (1)$$

Reactions due to impurities in the feed:

$$CaCO_3 + H_2SO_4 \text{ ---> } CaSO_4 + H_2O + CO_2 \quad (2)$$

$$SiO_2 + 4HF \text{ ---> } SiF_4 + 2H_2O \quad (3)$$

$$S + 2H_2SO_4 \text{ ---> } 2H_2O + 3SO_2 \quad (4)$$

Other possible reactions:

$$H_2O + SO_3 \text{ ---> } H_2SO_4 \quad (5)$$

$$HSO_3F + H_2O \text{ <---> } H_2SO_4 + HF \quad (6)$$

The heats of reaction at 1 atmosphere and 298.15 K are given in Table 5. At this stage in the design it can be assumed that all reactions except 6 go to completion. This assumes that the Fluorspar fed in sufficiently small particles and has sufficient residence time to ensure that mass transfer effects do not cause unreacted material to be lost. UK Patent No. 4,120,939 claims that temperatures of above 150 °C are needed to achieve fast reaction rates, a temperature which is also mentioned by European Patent No. 0096817, UK Patent No. 1,521,511, UK Patent No. 1,304,781, US Patent No. 3,278, 265 and US Patent No. 3,607,121. Raising the temperature increases the reaction rate but requires a move to more exotic materials of construction. Practically, the upper temperature limit is set by the boiling point of Sulphuric acid at the pressure of operation, if this pressure / temperature constraint is exceeded the reaction will cease as Sulphuric acid will no longer condense on the surface of the particles in order to react. In order to minimise the formation of Fluorosulphonic acid in the equilibrium reaction, 6, the temperature of reaction should be kept above 100 °C.

Table 5 - Heats of Reaction.

Reaction	Heat of Reaction
1	+69.8 kJ/mol CaF_2
2	+747.4 kJ/mol $CaCO_3$
3	-97.7 kJ/mol SiO_2
4	+253.8 kJ/mol S
5	-176.4 kJ/mol SO_3
6	-91.7 kJ/mol HSO_3F

All three options are effected in the same way by the additional compounds

introduced and by the by-product reaction, therefore the Level A rankings are unaltered.

4.5.3 Level C.

Running through the ten work stages at this level:

i) All three options include a reaction system, therefore they will all have a Reaction stage.

ii) The main reaction is the same in all cases. It is endothermic and must take place at elevated temperatures to attain reasonable rates of reaction, therefore heat will need to be supplied to the reacting system. The upper temperature limit is set by the boiling point of Sulphuric acid at the operating pressure, this is 330 °C for 100 % acid at atmospheric pressure. The lower limit is 150 °C, below which reaction rates drop below economically feasible levels. The temperature selected is a balance between rate of reaction and cost of materials of construction. An additional factor to be considered is that above 200°C the loss of H_2SO_4 with HF, causing a difficult separation, has to be taken into account. As processes with high conversion can be designed at atmospheric pressure there is no need to operate at elevated pressure. Pressures slightly in excess of atmospheric may be necessary to ensure safe operation by preventing the ingress of air.

iii) Within the operating conditions envelope the phases of the compounds present will be as follows:

Solid	CaF_2 and $CaSO_4$
Liquid	H_2SO_4 and Oleum
Vapour	HF, H_2O and SO_3

iv) The only feed that is in a different phase within the operating envelope than under atmospheric conditions is water, present only for Option 3. Pre-treating this in order to feed it as steam would further reduce the heat load on the reactor but this is not essential.

v) The reactions do not involve a catalyst therefore there is no reason to treat the feed to remove catalyst poisons. Only the Fluorspar contains significant levels of impurities and pre-treatment would not remove these. Therefore there are no additional reasons for pre-treatment.

vi) A separation section will be necessary in all cases to produce the required

product.

vii) The HF will leave the reactor as a gas but the product is required as a liquid, therefore the separation stage should include phase changing with a cold source. The $CaSO_4$ does not require a phase change but will need to be cooled.

viii) High conversion rates within the process mean that recycling to recover valuable raw materials is not necessary.

ix) Not applicable as there are no recycle streams.

x) Compounds produced in the reactions that are not product, HF, or by-product, $CaSO_4$, are SiF_4, H_2O, CO_2, H_2 and SO_2. All five will leave the reactor in the gas phase and their boiling points make all but water non-condensible without the use of refrigeration. Sulphur dioxide, at -10 °C, is second in order of descending boiling point. Water will be carried with the HF but waste treatment may be needed on the gaseous stream from the separation stage prior to disposal.

The outcomes of Level C are shown in Figure 9 and the number has increased due to the possibility of vaporising the water feed for option 3. At this stage, without equipment sizing, it is not possible to distinguish between options 3a and 3b in the economic rankings. Safety is discussed in Chapter 8. Due to space constraints only Option 1, with concentrated acid feed, will be considered from this point onwards.

4.5.4 Level D.

i) At this stage it will be assumed that the reaction is carried out at a pressure very slightly in excess of atmospheric and a temperature of 200 °C. To achieve high conversion rates on the F^- content of the feed the acid is fed slightly in excess. Working on the basis of a 20,000 Te/year plant producing HF with a maximum water content of 0.02 wt%, on line for 8,000 hours per annum, with the specified feed composition and reactions 1 to 4 all going to completion, the composition of the reactor outlet stream is as shown below with the corresponding feed streams. This assumes 1 mol % excess acid and that all unreacted acid leaves associated with the solid.

Product	kg/hr	Fluorspar	kg/hr	Acid	kg/hr
HF	2499.50	CaF_2	5008.38	H_2SO_4	6441.54
$CaSO_4$	8837.25	$CaCO_3$	77.00	H_2O	131.44
SiF_4	89.43	SiO_2	51.60		
H_2O	201.21	S	1.60		
H_2SO_4	63.86	H_2O	23.22		
CO_2	33.99				
SO_2	9.03				

The heat of reaction is +74.237 kJ/mol feed, equivalent to 1,385 kW. Additionally, specific heat will be required to raise the temperatures of the feeds from ambient to 200 °C and latent heat will be consumed during the evaporation of the water in the feed. These requirements amount to 814 kW, giving a total reaction stage heat load of 2199 kW.

ii) The reaction will be heterogeneous, with the Sulphuric acid condensing on the surface of the solid Fluorspar, and is endothermic so that both mass and heat transfer effects need to be taken into account in the design of the reactor. These will be dominated by the size of the Fluorspar particles fed and the residence time within the reactor. If particles are too large then the material at the centre will be carried through the reactor unchanged and there will be a loss of F^-. Conversely if they are too small there will be a tendency for them to be carried out of the reactor in the gas stream. European Patent No. 0096817 gives a preferred average particle size of 40 to 80 microns. It is assumed that acid grade Fluorspar within this size range is readily available and that it will not be necessary to include crushing facilities.

iii) The reactor selected has to be capable of handling a liquid reacting on solid particles and evolving a gas. Additional features required are the ability to give sufficient residence time for mass transfer effects to be overcome and the need to add heat into the reacting mass. An added complication is that the reacting mass passes through phases where it becomes pasty and difficult to handle, coating process equipment. Heat transfer through the crust makes it difficult to maintain the reacting mass at a sufficiently high temperature. Maintaining a thin layer of crust can protect materials of construction. UK Patent No. 2159136 claims that a system where a pre-reactor is used to achieve a conversion of 40 to 50 % followed by a main reactor

with recycle of solid product to give an inlet conversion of 70 to 80 % avoids these handling problems. Figure 10 shows the six possible reaction schemes. The simplest is option A with only a single reactor, the disadvantage of this simplicity is that the system would be difficult to operate and maintain due to caking. Option C uses a recycle of solid material to give a feed to a single reactor with 70 to 80 % conversion in order to overcome some of the handling problems. This system still has a risk of block formation at the inlet which would limit yield and would require an increase in reactor size in order to handle the recycle flow. Option B uses a premixer to overcome the problem of block formation, but as this is unheated the conversion at the outlet would be limited to 25 to 30 % and there would still be handling problems within the main reactor. Option D refines option B to avoid the majority of handling problems by using solid recycles to both the premixer and main reactor feeds. This would result in increases in size for both the premixer and main reactor. Options E and F use a heated pre-reactor to overcome initial handling problems. Option E would have residual handling problems in the main reactor which option F overcomes by the inclusion of a recycle stream. The balance is between ease of material handling, affecting operability and maintainability, and equipment size and complexity, affecting economics. This balance cannot be fully explored without undertaking equipment sizing, requiring all options to be carried forward to Level F.

The most frequently used type of main reactor is a rotary kiln where the residence time is dictated by the length, speed of rotation and angle of inclination. Of these factors only the speed of rotation can be altered once the plant has been built. To achieve a complete reaction a residence time in excess of 60 minutes is required. Heating of a rotary kiln is usually from a jacket containing steam or hot combustion gases. Given the reactor heat load and the need to condense the outlet gases prior to treatment the possibility of using heat recovery to increase energy efficiency should be considered. Flights within a rotary kiln rapidly corrode and need frequent replacement, particularly if there is only a single reactor. Also in this case the inclusion of wall scrapers to reduce caking is necessary, old railway rails have been used for this purpose. Other possible main reactor types are fluidised beds, only if using Option 3 and a free-fall stationary type, discussed by US Patent

No. 4,120,939 and US Patent No. 3,469,939. These are relatively unproven in an industrial situation.

Essentially the same type of equipment is needed for a premixer or pre-reactor but with the latter requiring some means of inputting heat, usually via a jacket. A simple stirred tank can be used but the stirrer tends to require frequent replacement. An alternative is to use a static mixer but careful consideration must be given to the removal of HF gas in the case of the pre-reactor and the need to achieve a residence time of 30 minutes. The residence time required results in premixer and pre-reactors of considerable size and cost.

iv) No feedstock pre-treatment is necessary.

v) Some of the alternative reaction schemes discussed above use a recycle of solid material in order to improve the flow characteristics within the reaction system. These streams would require the conveying measures, which could be integral with the reactor if a rotary kiln is used.

Using the following cost information the economic potential at this level can be estimated. This does not take into account any losses in waste streams, considered during the next level, or assign any value to the non-condensible gas stream.

HF	£911 /Te (0.02 wt% water)
$CaSO_4$	£105 /Te (Sales limited to 20,000 Te/yr)
Fluorspar	£140 /Te
H_2SO_4	£53 /Te (98 wt%)

Feedstock costs = 8,568,160 £pa

Product revenue = 20,320,000 £pa

Economic potential = 11,751,840 £pa.

These figures are sufficiently attractive to continue considering this alternative.

4.5.5 Level E.

HF and water form an azeotrope with a boiling point of 111.4 °C and a composition of 35.6 wt% HF. The water content of the stream exiting the reactor is on the HF side of the azeotrope. The product specification to be met is a

maximum of 0.02 wt % water, therefore there is no need to break the azeotrope. No other azeotropic data was uncovered for substances within the system. It would therefore appear that the required separations will be possible without a need to considering altering the reactor outlet conditions.

i) Considering the reactor product stream given in stage i of Level D the destination of the components is as follows:

Component	Destination
HF	Product
$CaSO_4$	By-product and Waste (solid)
SiF_4	Waste (gaseous)
H_2O	Product and Waste (gaseous)
H_2SO_4	By-product and Waste (solid)
CO_2	Waste (gaseous)
SO_2	Waste (gaseous)

ii) As discussed previously there is a need to condense the reactor gaseous outlet stream in order to produce liquid HF. This could be done in a single step using cooling water but for additional recovery of HF this could be followed by the use of a refrigerated system. This would introduce cost and have a SHE impact due to the use of the refrigeration medium. At lower temperatures an increased amount of SO_2 would pass into the liquid system and require removal from the product.

iii) The reactor produces a solid and a gaseous outlet stream. These exit the reactor separately and there is no need to include additional phase splitting equipment to separate them. Phase separation will be necessary for the condensed gas stream.

iv) As the gaseous streams are not recycled there is no need to consider the need for purging. The stream should be treated in such a way that when released to atmosphere it conforms to the applicable environmental limits. Simple technology such as a two stage scrubbing process using Sulphuric acid followed by water would achieve this. Acid washing medium would be fed to the reactor to minimise waste production. The waste stream from the water scrubber would require neutralisation prior to disposal. Other combinations of scrubbing medium could be used but the integration with the process would be lost.

v) As there is no need to break an azeotrope, a simple distillation unit

operation will be sufficient to achieve product specification. The HF will be the top product and the bottoms will include Water, some Sulphuric acid and traces of other reactor outlet components. Treatment to neutralise this stream will be necessary prior to disposal and may be carried out in conjunction with that for the water scrubber waste, if this unit operation is present.

vi) Feeding an excess of acid means that the $CaSO_4$ stream will require to be treated with an alkaline substance to ensure that it is neutral prior to removal for sale or landfill. This could be via the use of chemicals such as NaOH or by steam stripping to remove the acid. The first requires the use of an additional hazardous chemical that must be purchased and handled but does not produce a waste stream. The second has an associated energy cost and produces a weak acid stream that must be disposed of. Without concentration it is unlikely that this stream could be recycled. From an environmental point of view the first option would be preferred. The safety impact of handling caustic soda can be mitigated by utilising industry standard methods.

viii) Emission limits are site specific and cannot be stated for a generic plant. Four waste streams have been identified for the plant, CaF_2 for which there is no market, Non-condensible material produced in the reactor, Scrubbing effluent and Distillation bottoms. The principles of waste minimisation have been captured in the design and there are no further possibilities for reduction. Neutralisation and scrubbing are the identified treatment processes.

A sample flowscheme produced at Level E is shown in Figure 11.

4.5.6 Level F.

Due to space limitations process design work will only be briefly mentioned. The focus is on problems encountered. Some problems were encountered when undertaking this work due to the none conventional nature of the reactor systems being investigated. It is felt that if this work had been carried out for anything other than a small number of alternatives then the burden of work would have been too great. The focus should be on exploring possible alternatives and recording those uncovered fully, but only progressing the design of a small number that seem most promising. Without the economic and business framework of an industrial design

this type of work is difficult to mirror in an academic environment.

4.5.7 Level G.

As only a single option was carried past Level C this level cannot be meaningfully included in a report of the case study.

4.6 Conclusions

Key to the success of any design methodology is the ability to flexibly address a wide range of project types. Flexibility must include allowing users a certain degree of freedom in choosing their point of entry into and route through the method. Imposing a very rigid working structure should be avoided at all costs as this will discourage use. Using the proposed methodology it was found to be easy to rapidly develop and explore a number of possible alternative flowschemes, perhaps too easy as the quantity of work in progressing and recording adequately more than two or three designs is considerable. Focusing on "best guess" designs and recording the history of others to allow back tracking is seen as the most efficient way of working. The capturing of design history is covered in Chapter 6.

Table 1 - Comparison of levels included in the models due to Douglas and the proposed model.

Douglas 1988	Douglas 1992	Proposed Model
Level 1 - Input information and Batch versus Continuous **Level 2** - Input-Output structure of the flowsheet **Level 3** - Recycle structure of the flowsheet **Level 4** - General structure of the separation system 4a - Vapour Recovery System 4b - Liquid Recovery System **Level 5** - Heat exchanger network	**Level 1** - Input information : type of problem **Level 2** - Input-Output structure of the flowsheet **Level 3** - Recycle structure of the flowsheet **Level 4** - Specification of the separation system 4a - General structure: phase splits 4b - Vapour Recovery System 4c - Liquid Recovery System 4d - Solid Recovery System **Level 5** - Energy Integration **Level 6** - Evaluation of alternatives **Level 7** - Flexibility and control **Level 8** - Safety	**Level A** - Main route alternatives **Level B** - Definition of reaction system **Level C** - Processing stages **Level D** - Production definition **Level E** - Treatment definition **Level F** - Basic process design **Level G** - Screening

Table 2 - Framework proposed by (Mansfield and Cassidy 1994).

Decision Point	Key Questions/Decisions	Information Used
Initial Specification	What Product? What Throughput?	Market Research R&D new product ideas
Process Synthesis Route	How to make product? What route? What reacting materials? Starting point?	R&D Chemists research Known synthesis routes and techniques
Chemical Flowsheet	Flowrates, conversion factors, basic unit operation selection, temperatures, pressures, solvents and catalyst selection	Process synthesis route Laboratory and pilot scale trials Knowledge of existing processes
Process Flowsheet	Batch versus Continuous operation Unit operation selection Control/ operation philosophy	Information above plus: Process engineering design principles and experience
Process Conceptual Design	Equipment selection and sizing Inventory of process Single versus multiple trains Utility requirements Over design/ Flexibility Recycles and buffer capacities Instrumentation and control Location / siting of plant Preliminary plant layout Materials of construction	As above plus: Equipment supplies data, raw materials data, company design procedures and requirements
Process Detailed Design	Detailed specification based on conceptual design	Process conceptual design and codes / standards Experience on past projects / designs

Figure 1 Initial MEK Block Flow Diagram

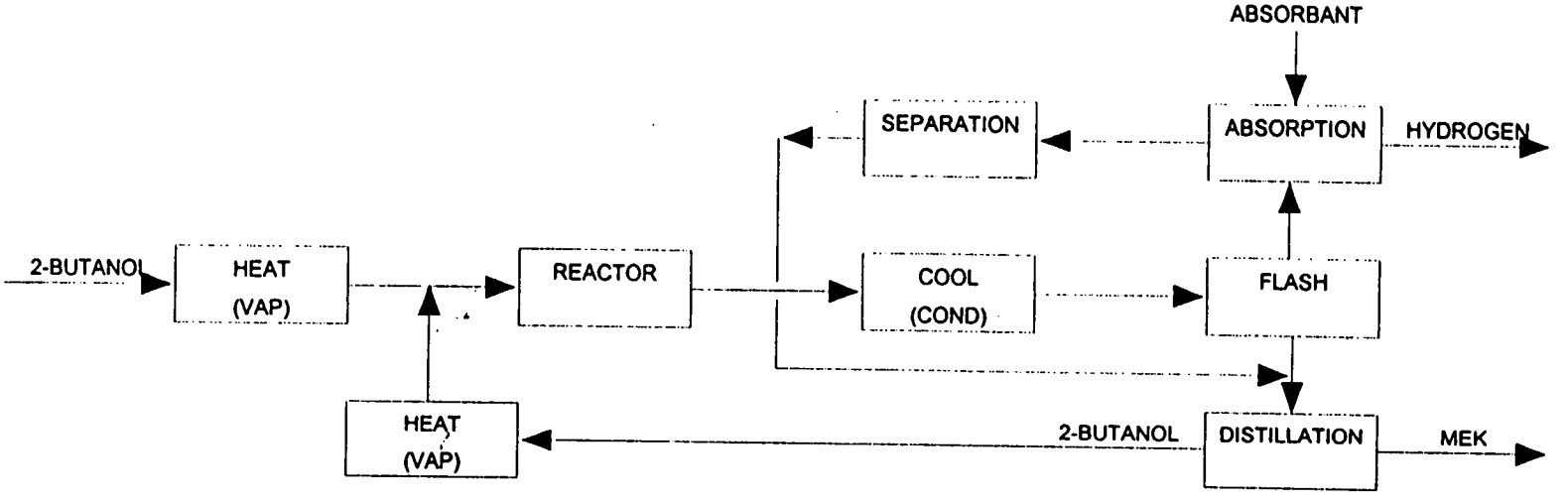


Figure 2 Level 2 Starting Point

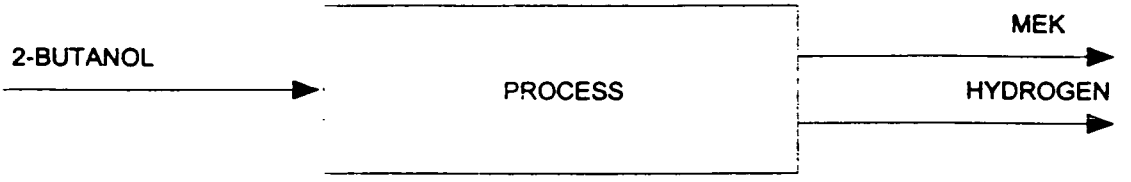


Figure 3 Level 2 Outcome

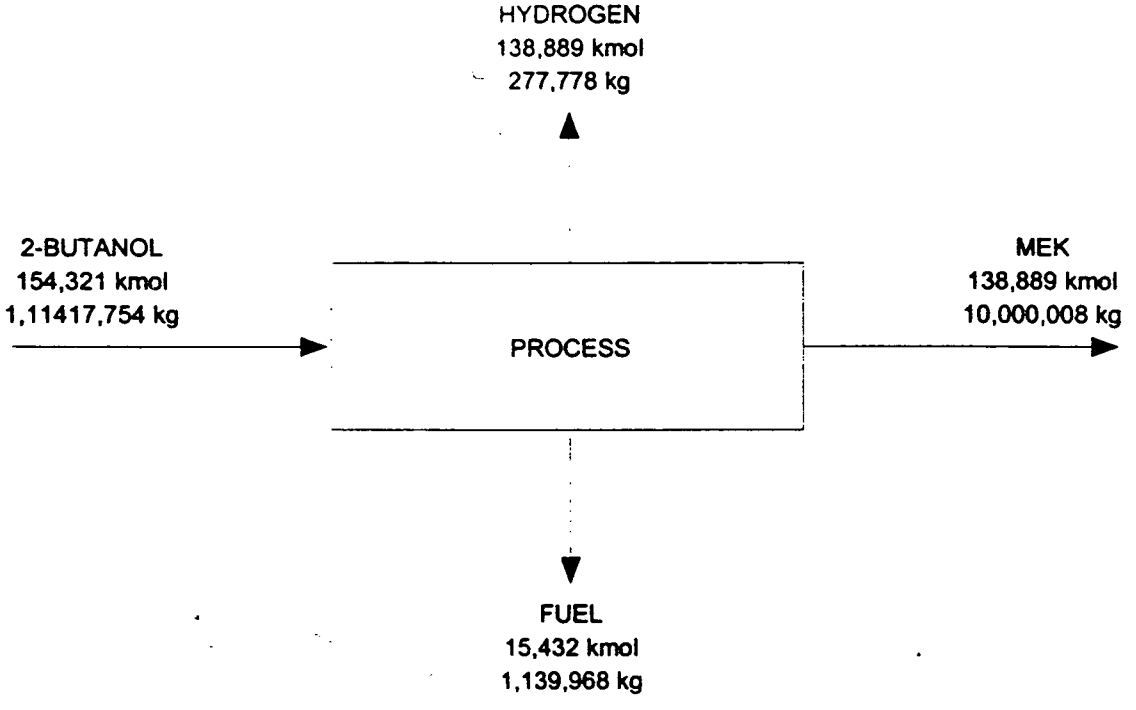


Figure 4 Level 3 Outcome

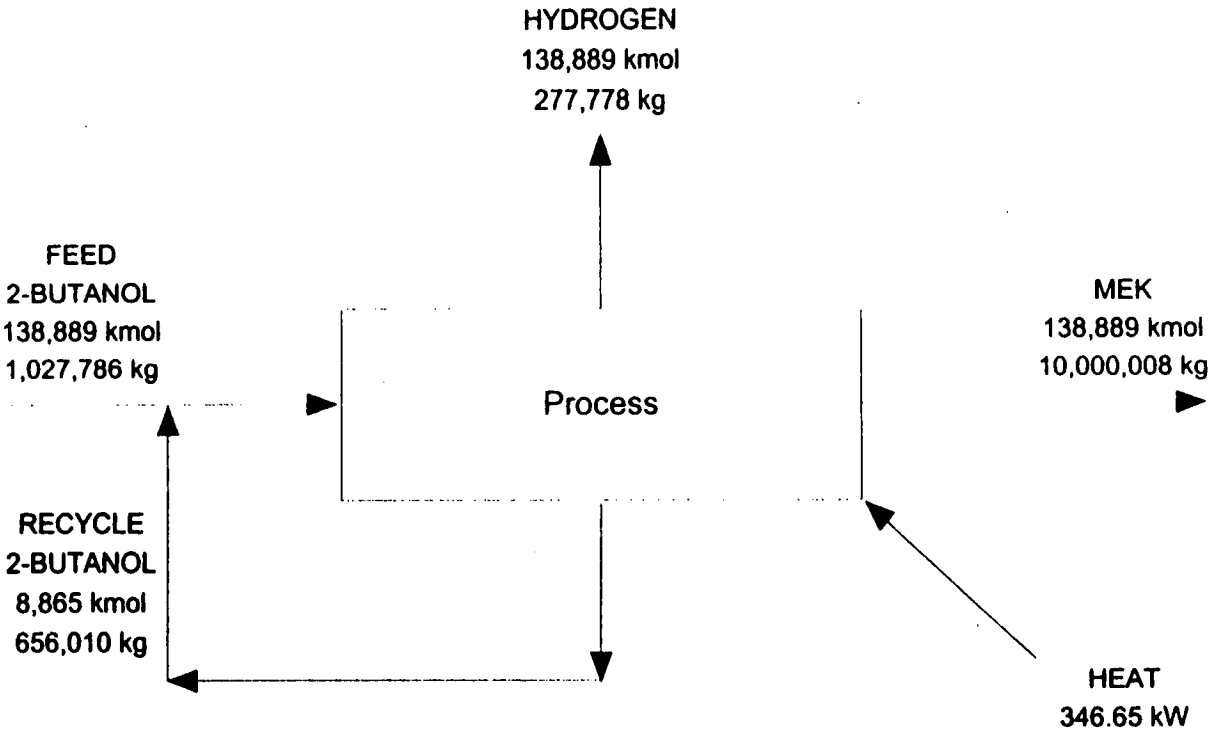


Figure 5 Initial Separation System Structure

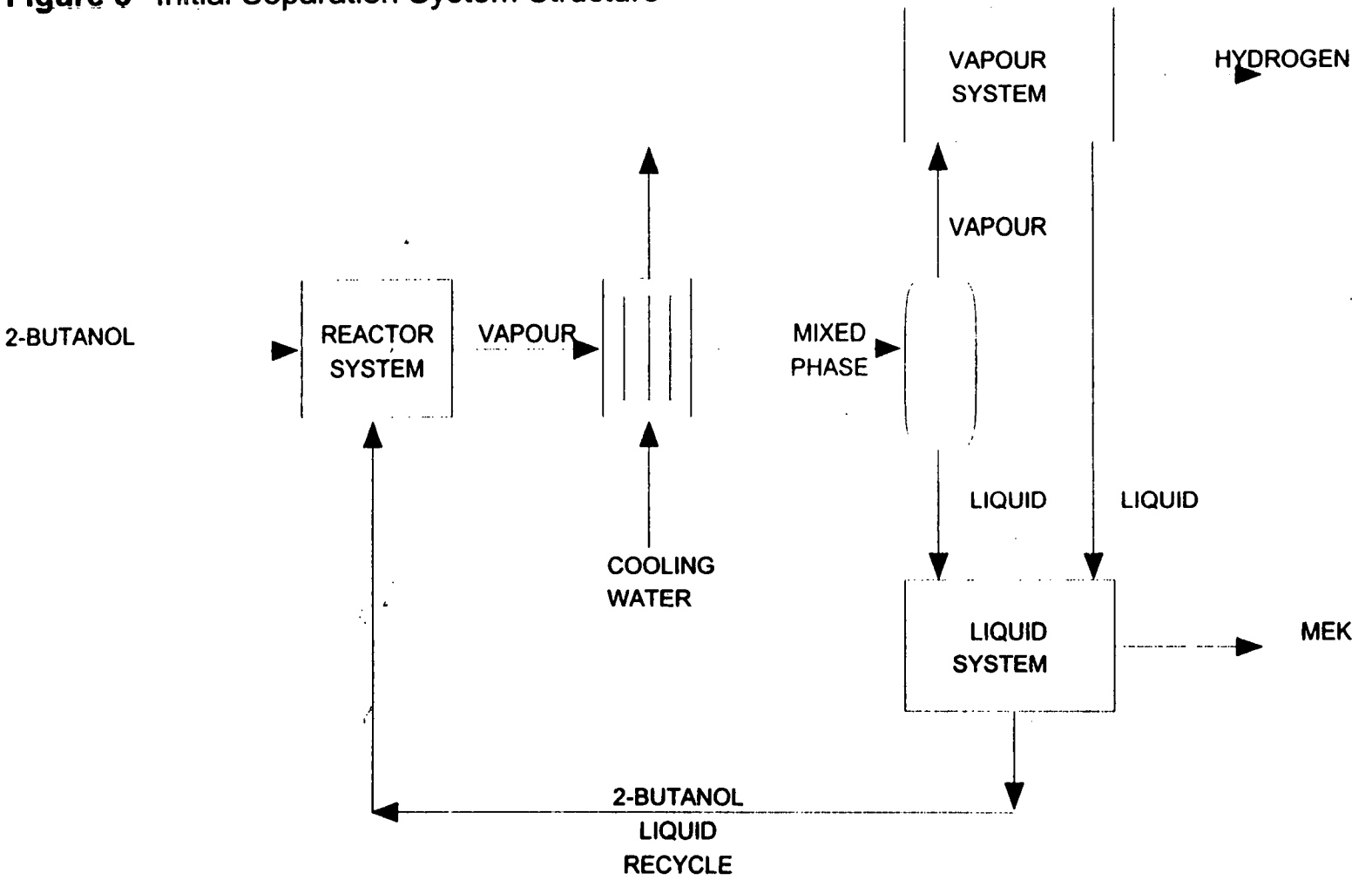
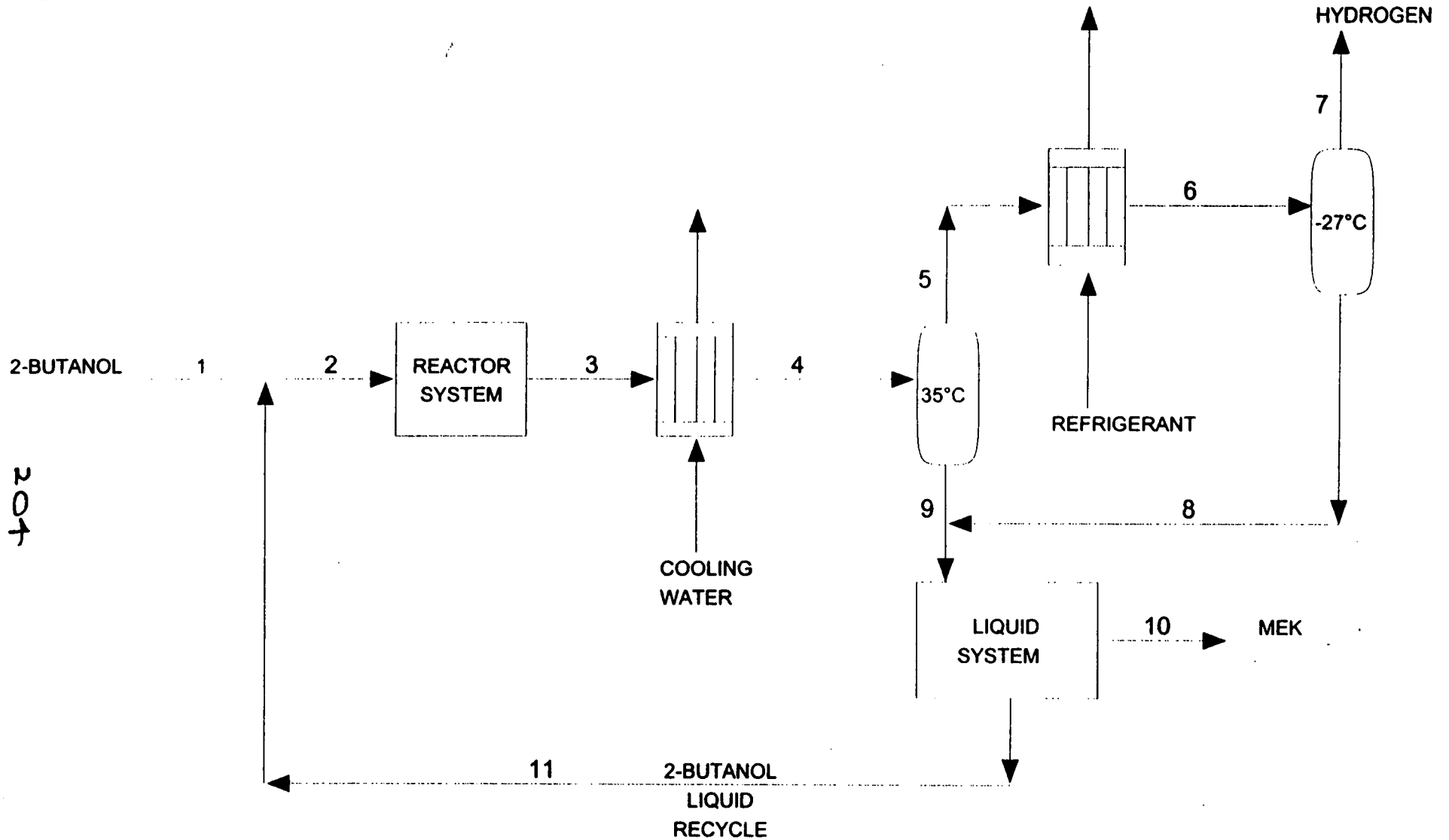


Figure 6 Level 4, Part 1 Outcome

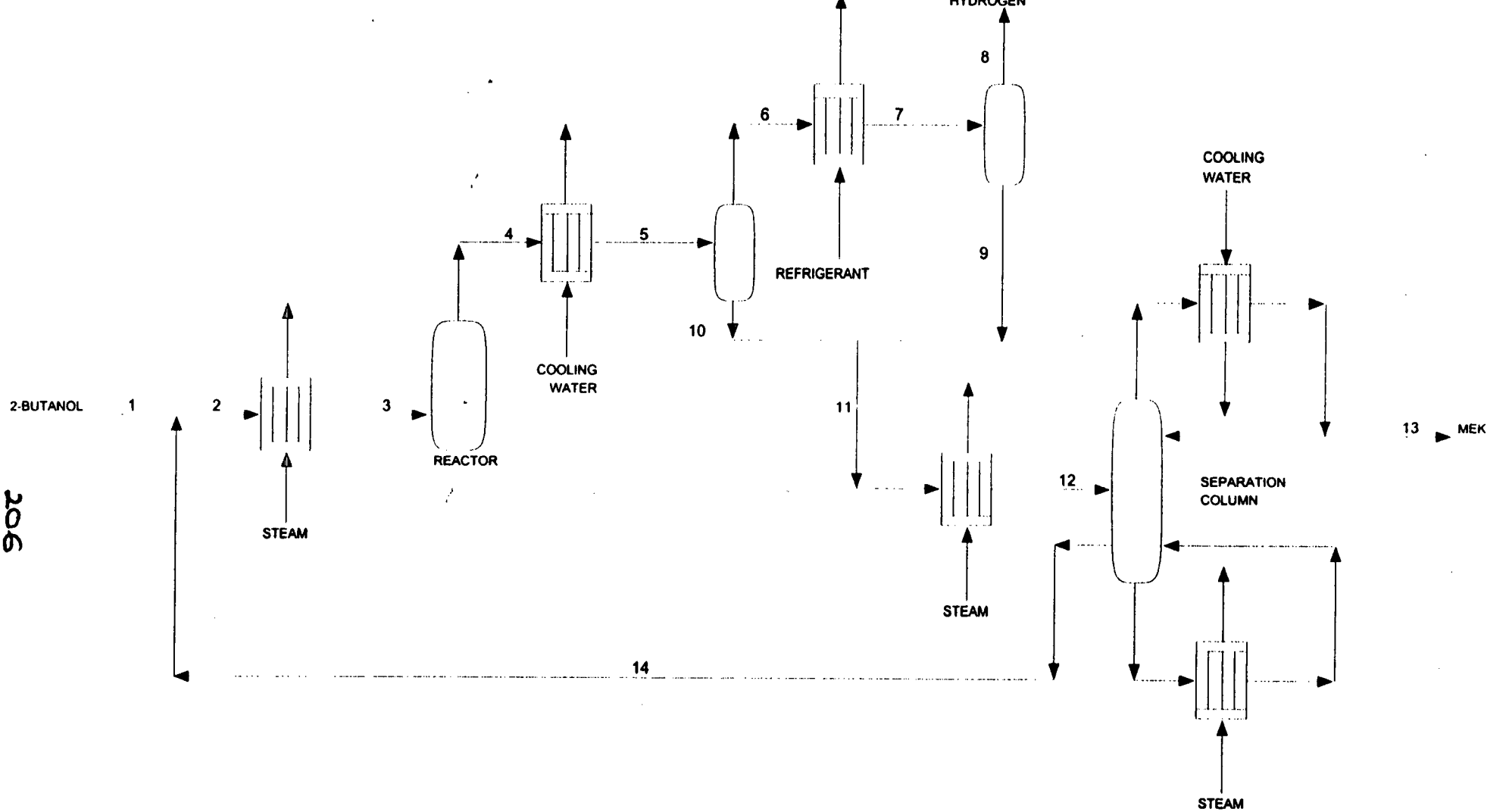


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Table 4 Level 4, Part 1 Outcome Mass Balance

Component	1 kg/hr	1 kmol/hr	2 kg/hr	2 kmol/hr	3 kg/hr	3 kmol/hr	4 kg/hr	4 kmol/hr	5 kg/hr	5 kmol/hr	6 kg/h	6 kmol/hr
Hydrogen	----------	----------	----------	----------	35.2542	17.6271	35.1597	17.3798	35.1468	17.5734	35.1468	17.5734
MEK	----------	----------	----------	----------	1257.6435	17.4673	1257.6435	17.4673	165.7418	2.3020	165.7418	2.3020
2-Butanol	1290.3470	17.4371	1373.0378	18.5546	82.7181	1.1178	82.7181	1.1178	3.9858	0.0539	3.9858	0.0539

Component	7 kg/hr	7 kmol/hr	8 kg/hr	8 kmol/hr	9 kg/hr	9 kmol/hr	10 kg/hr	10 kmol/hr	11 kg/hr	11 kmol/hr
Hydrogen	35.1459	17.5730	0.0009	0.0005	0.0129	0.0064	0.0138	0.0069	----------	----------
MEK	7.6369	0.1061	158.1050	2.1959	1091.9016	15.1653	1250.0000	17.3611	----------	----------
2-Butanol	0.0272	0.0004	3.9587	0.0535	78.7321	1.0639	----------	----------	82.6908	1.1174



STREAM	1	2	3	4	5	6	7	8	9	10	11	12	13	14
PHASE	LIQUID	LIQUID	GAS	GAS	MIXED	GAS	MIXED	GAS	LIQUID	LIQUID	LIQUID	B.PT.	LIQUID	LIQUID
HYDROGEN				35.1597	35.1597	35.1468	35.1468	35.1459	0.0009	0.0129	0.0138	0.0138	0.0138	
MEK		0.7079	0.7079	1257.6435	1257.6435	165.7419	165.7419	7.6369	158.1050	1091.9016	1250.0066	1250.0066	1249.2987	0.7079
2-BUTANOL	1291.6380	1361.7234	1361.7234	82.7180	82.7180	3.9859	3.9859	0.0272	3.9587	78.7321	82.6908	82.6908	12.6054	70.0854
TEMP. °C	20		400	320	35	35	-27	-27	-27	35	28	62		

Figure 8 Level A Alternative Schemes

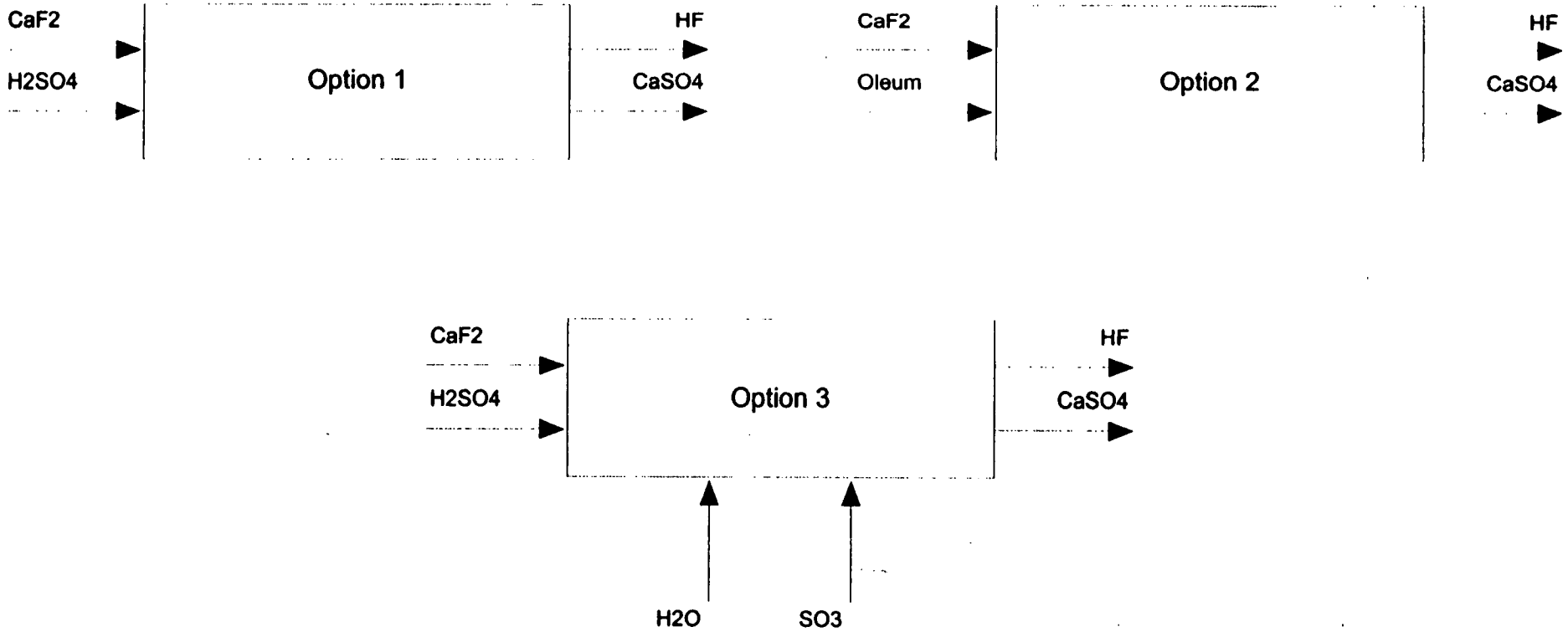
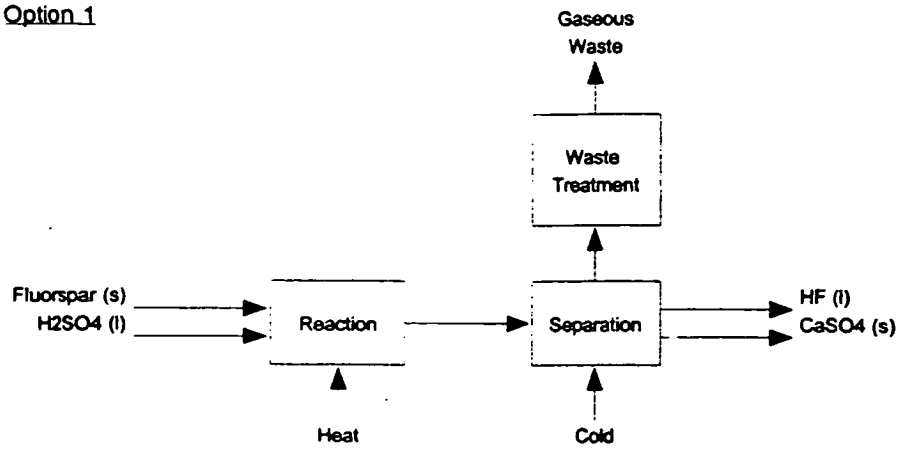
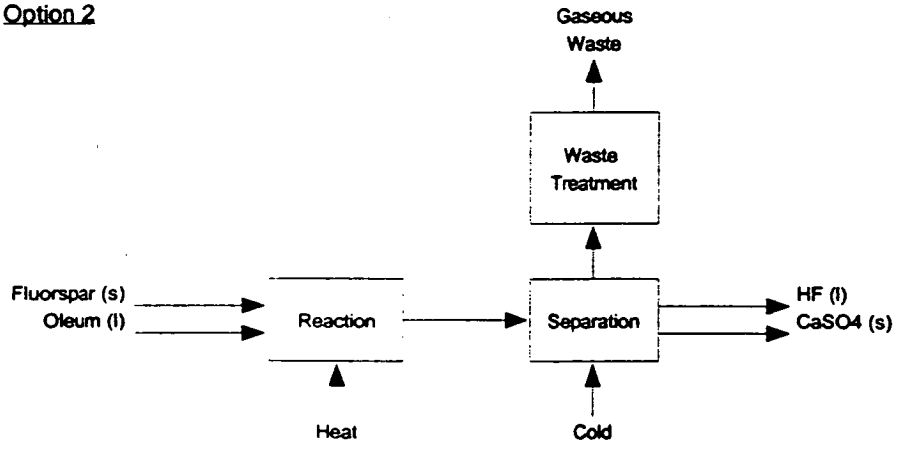


Figure 9 Level C Alternative Schemes

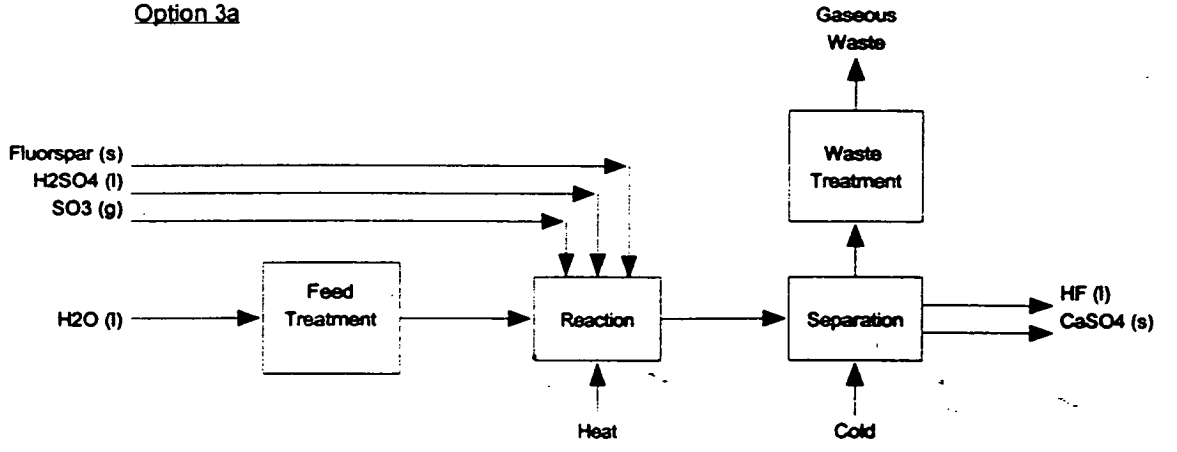
Option 1



Option 2



Option 3a



Option 3b

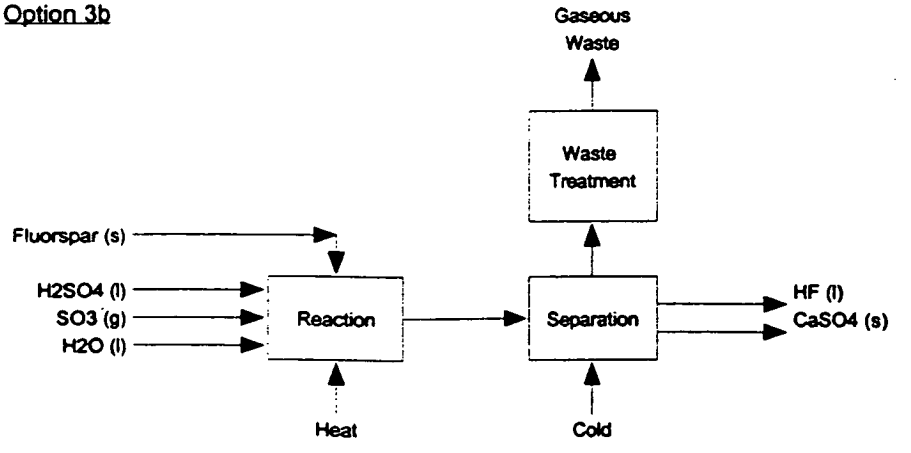
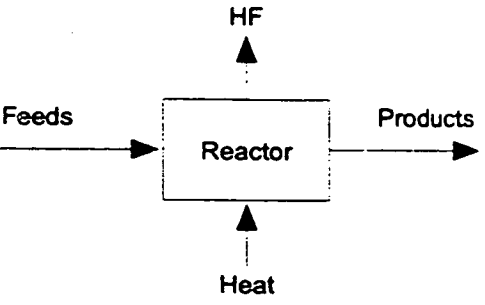
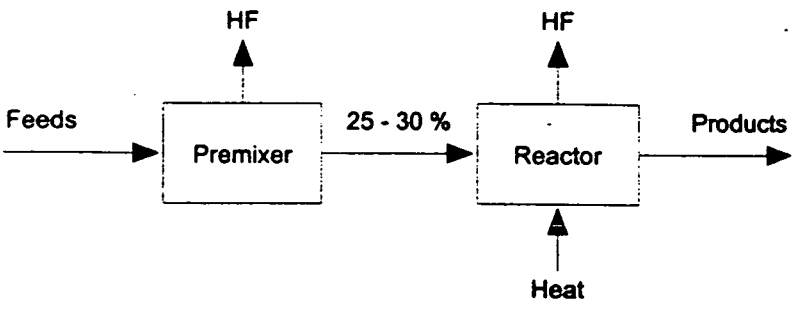


Figure 10 Level D Reactor Scheme Layouts.

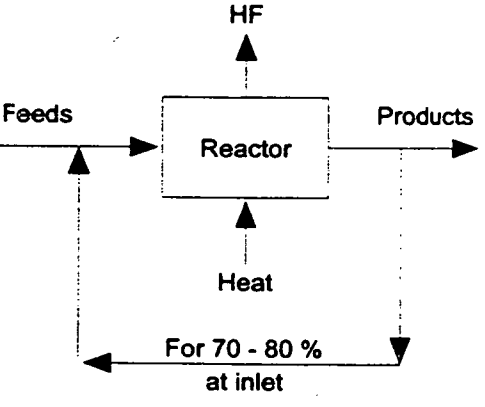
Option a Single Reactor



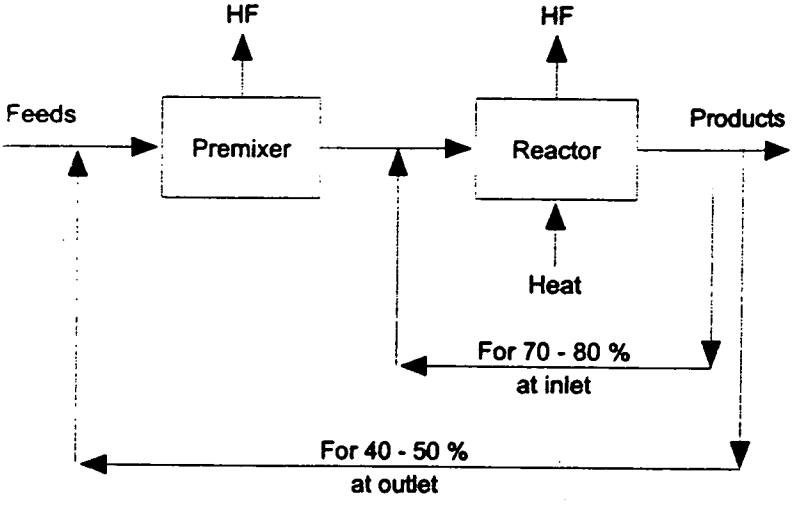
Option b Reactor with Premixer



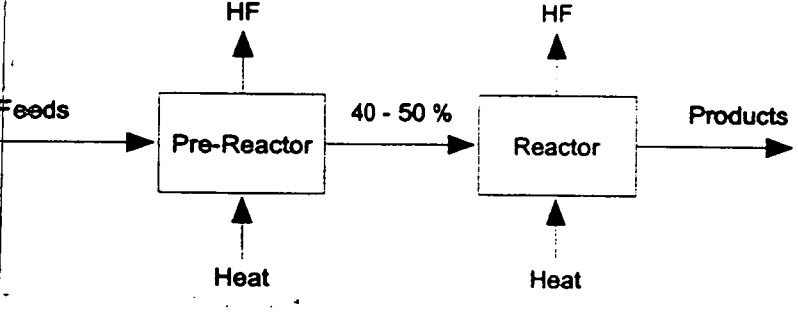
Option c Single Reactor with Recycle



Option d Reactor with Premixer and Recycle



Option e Reactor and Pre-Reactor



Option f Reactor, Pre-Reactor and Recycle

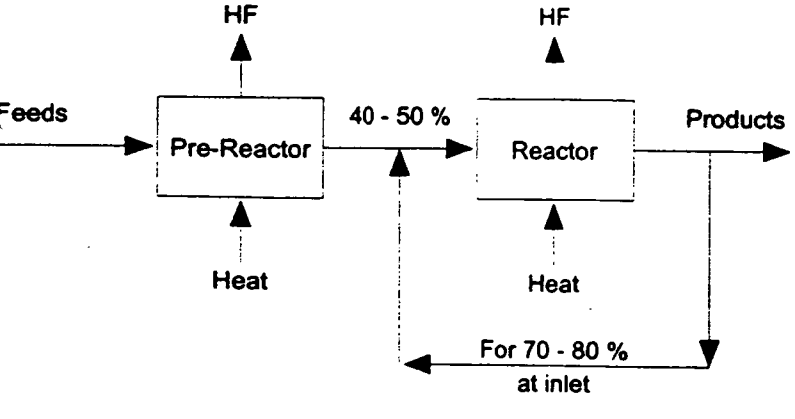
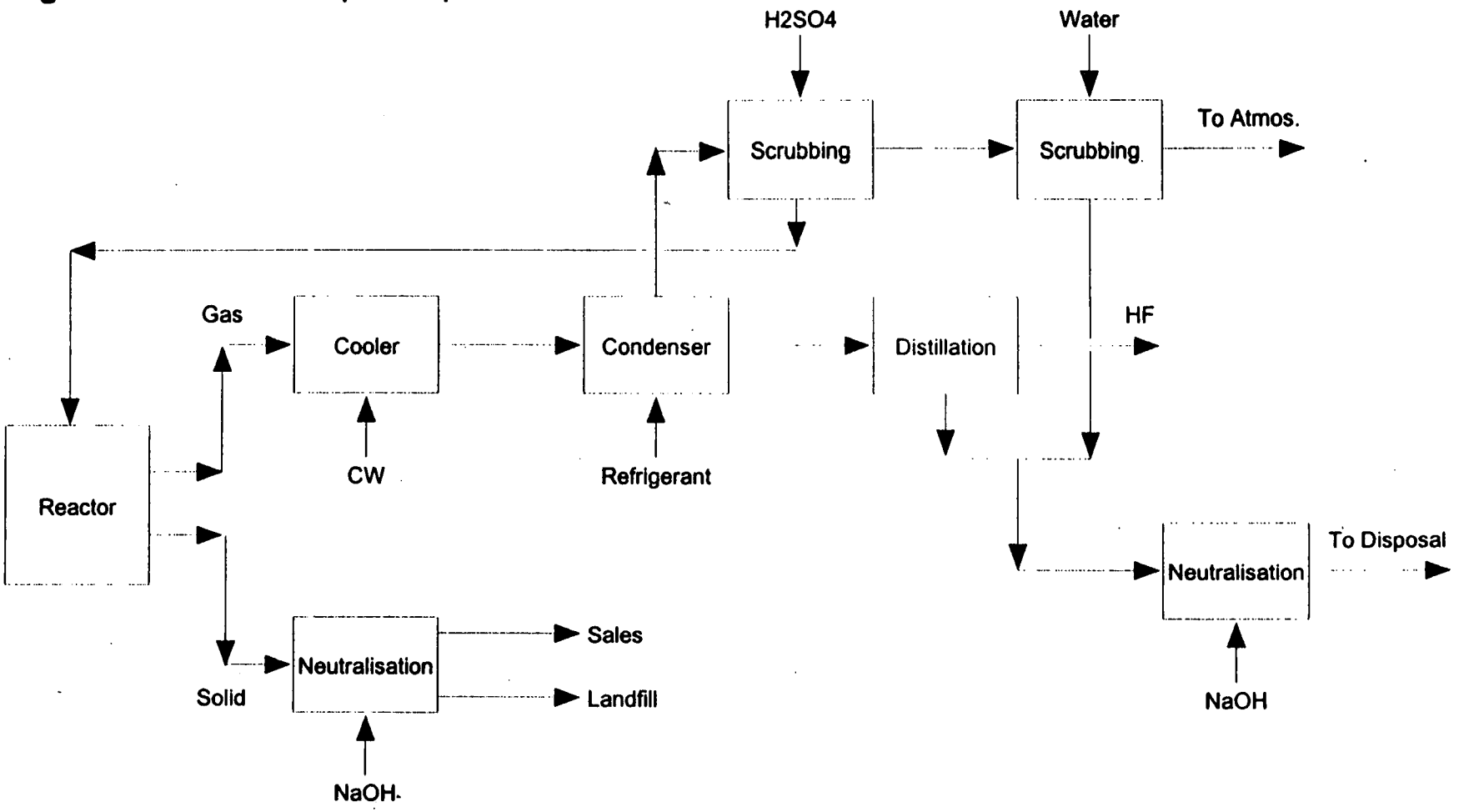


Figure 11 Level E Sample Output



Chapter 5

Use of CHiPS

5.1 Introduction

Process synthesis can be defined as the step in design where the component parts of a plant are selected and interconnected. With synthesis the required outputs are specified and the inputs are specified or given an allowable range and the task is to generate the optimum process. When the inputs and the process are known the outputs are generated by analysis. Malone and Doherty point out that both synthesis and analysis are necessary before design, where the inputs, process and outputs are known, can be undertaken, (Malone and Doherty 1980). The primary result of this step is a flowsheet of the process. However, as there are many possible flowsheets that could produce the desired product from a given starting point an important part of the design process is, as discussed in Chapter 4, the generation of alternatives. To aid the designer, synthesis tools that suggest a number of different solutions to a problem input by the user can be used to generate possible solutions that may not have been generated by the user alone. Work in this area has been ongoing for some years with a disappointingly slow uptake into main stream computer aided design. Gregory and Bridgewater discuss work undertaken in the early 1970s in this field, (Gregory and Bridgewater 1972). They cover work to extend an alternative generation and evaluation scheme in the field of minerals processing into the area of chemical process synthesis. Ranking of alternatives was purely by economic means. Mahalec and Motard saw the improvement of the innovative capacity of engineers as being the most significant potential for synthesis, (Mahalec and Motard 1977). To aid this Johns and Romero propose a simplified synthesis method for use during the early stages of design, (Johns and Romero 1979). Details of concentration levels are omitted along with heat integration. These factors are considered to be unimportant initially and are reserved for consideration at a later stage. The low level of detail leads to rapid computation. As the number of possible solutions to a design problem is large it is necessary for simulation tools to undertake ranking

before presenting the user with the results of the synthesis. There are 1134 simple, sharp separation sequences possible for the separation of five components using three technologies, (Nishida et al 1981). At this level it would not be possible for a designer to take in and assess the quantity of information available. The most commonly used form of ranking indicator is based on some form of economic factor such as annualized cost. A number of the synthesis tools discussed in this chapter concentrate on presenting the user with a single solution, usually optimised with respect to cost, which completely removes the designer from the decision making process. There is a balance to be struck between this position and presenting the user with so many alternatives that the manual screening process becomes extremely time consuming. CHiPS addresses this point by allowing the user to specify the number of ranked solutions that are to be presented.

A large volume of work exists on synthesis and a number of review articles have been published. Westerberg presented such a review at a meeting claimed to be the first to discuss computer applications in Chemical Engineering in America, (Westerberg 1979). He cites two earlier reviews, published in 1973 and 1978, and lays down the format for the subsequent reviews. Nishida and co workers present an overview of the first decade of progress in this area and point to the work by Rudd and his students in developing AIDES (Adaptive Initial DEsign Synthesizer) as being the starting point, (Nishida et al 1981). Siirola and Rudd describe the synthesis principles behind AIDES and the initial computer implementation using a teletype terminal, (Siirola and Rudd 1971). Twelve alternating synthesis and analysis steps of increasing complexity were used as the basis, of which nine, covering from the reaction path stage to the synthesis of the process task network, were implemented in AIDES. The twelve stages used are as follows:

(i) Synthesis Step 1: Chemical Reaction Path. A sequence of chemical reactions synthesised by research chemists.

(ii) Analysis Step 1: Stoichiometric Material Balance. Estimates of raw material usage and amount of product made, based on estimated reaction conversions, used to determine the preliminary economic feasibility.

(iii) Synthesis Step 2: Component Matching. Sources and destinations of material species are used to map the possible material routes through the

process.

(iv) Analysis Step 2: Match Evaluation. Possible mapping through the process are evaluated.

(v) Synthesis Step 3: Species Allocation. Routes for all the species present are determined.

(vi) Analysis Step 3: Information Difference Detection. Differences in values of variables along the routes that make up the process are used to determine where unit operations are likely to be required.

(vii) Synthesis Step 4: Non-separation Task Identification. The first step to specify unit operations to clear information differences.

(viii) Analysis Step 4: Physical Property Evaluation. Physical property differences are explored to determine the possible separation unit operations.

(ix) Synthesis Step 5: Separation Task Identification. Synthesis of the possible separation sequences.

(x) Analysis Step 5: Separation Task Feasibility. Evaluation of the possible separation sequences.

(xi) Synthesis Step 6: Task Integration. Selection of equipment to carry out the selected route.

(xii) Analysis Step 6: Final Evaluation. Process design of the selected route or routes.

As discussed by Siirola and Rudd AIDES implements the above steps up to analysis step 5.

AIDES was followed by BALTAZAR, by Mahalec and Motard. Both used heuristics and linear programming and did not include equipment costing. Grossmann and Daichendt provide an updated review, (Grossmann and Daichendt 1996). The work on the process synthesis problem can be split into the following sections. These are the key elements in the decomposition of the synthesis problem into "manageable" chunks.

(i) Synthesis of reaction paths

(ii) Synthesis of separation sequences

(iii) Heat exchanger network synthesis

(iv) Reactor network synthesis

(v) Chemical process synthesis

(vi) Synthesis of control structures for chemical processes

Hlavácek provides an early review of work in this area, (Hlavácek 1978), and identifies Rudd as the originator of such process design decomposition. Stephanopoulos points to 1968 as the start of active work on synthesis and states that 250 - 300 research articles, 7 review articles and 3 books had been published in the period to 1980, (Stephanopoulos 1980). Umeda attempts to give an overview of process synthesis, including a review of reviews, (Umeda 1983). He focuses on the large body of work that has been undertaken in Japan. Given the importance that such activity would appear to attach to synthesis it is disappointing that general acceptance and use of the resultant techniques is still at a relatively low level. Umeda advocates the approach of linking synthesis to project stages to aid uptake.

There are two main approaches to synthesis: evolutionary, which begins with an existing flowsheet and seeks to improve it, and generative, where no initial flowsheet exists. Evolutionary problems can be approached by traditional process design techniques or by the use of a structural parameter approach. The quality of results from any evolutionary technique is strongly dependent on the solution used as the starting point. Typical of this approach is work by Douglas. Heuristics for separation system synthesis are discussed in (Douglas and Stephanpoulos 1994) along with a discussion of the automation requirements for a heuristic based system. Heuristic methods can be viewed as a means of generating this starting point. Evolutionary rules can then be used to challenge the structure generated by challenging the heuristics upon which it was based. Such a system, using eight heuristic rules to generate the initial solution and five evolutionary rules to refine it, is proposed by (Nath and Motard 1981). Here optimisation is with respect to annual cost. An alternative approach is to use algorithmic methods. These are in principle rigorous but due to limitations in computational times the search space is usually limited by heuristics or bounding. Algorithmic methods rely on the use of standard non-linear solution techniques to produce a result. There are a number of different

approaches to generative problems. These fall into two general categories: systematic generation and superstructure optimisation. The first builds a flowsheet from smaller, more basic components and the second starts with a large superstructure containing many alternatives and applies optimisation. Here the main drawback is that unless all alternatives can be guaranteed to be included within the superstructure then the optimal solution may not be found.

One approach to systematic generation is to develop methods based on the elimination of property differences between the initial and, desired, final states. Whilst some elimination steps are closely tied to unit operations this is not simply an exercise in bolting together unit operations. Siirola gives a discussion of property difference methods and mentions three problem areas, Siirola 1994):

(i) Certain property changing methods can only be applied when other properties already have specific values.

(ii) A difference may not be entirely eliminated by a method.

(iii) It is necessary to establish a hierarchy of methods to tackle property differences to avoid conflict.

Alternatives are generated when more than one possible property change method is available to eliminate a difference. Recycle streams identified during the design may result in the need for iteration if the properties of the recycle streams alter the property differences to be resolved. Little has been published on the property elimination approach to synthesis other than by Siirola, who is industry based. Is this because it does not represent a sufficiently elegant mathematical problem or because the approach would not work? A more general approach of this type is to systematically eliminate differences between start and goal states. Work on this basis is described by (Mahalec and Motard 1977). They define the synthesis problem as follows:

Given a set of chemical reactions, a set of elementary physical processing operations and a set of available raw materials select a subset that will achieve a subset of the products of interest.

To aid solution the problem is decomposed into steps related to selection from

each of the sets with heuristics used as appropriate. The system proposed by Mahalec and Motard sequentially looks at each of the goals but considers all species within these goals simultaneously. The AIDES system adopted a similar decomposition approach but considered each species at a time. In both cases the choice of operations available was limited to fundamentals such as mixing, separation, reaction and change in pressure. Hlavácek identifies two procedures for generative methods; General Problem Solver (GPS), as used by the AIDES programme, and Mechanical Theorem Proving (MTP), as used by Motard and co workers, (Hlavácek 1978). GPS begins with a set of facts and attempts to derive the goals or conclusions. TP begins with the goals and attempts to demonstrate the consistency with the given facts. This approach type would dovetail well into an hierarchical design procedure and the alternatives generated could be tracked by KBDS.

For the superstructure optimisation category breadth- and depth-first tree-search methods involve exploring the interconnections between nodes but involve prohibitively high computational times as the size of the synthesis increases. Consequently these methods are usually combined with heuristic or bounding methods. The first of these is based on the experience of the process engineer undertaking the design but carries no guarantee of optimality. Of bounding methods one of the most successful has been the branch and bound algorithm. The final method for generative problems is decomposition where the design is subdivided into problems that can then be solved more easily. The advantages and disadvantages of each method and combination of methods will not be discussed here. Flowers and co workers present a distillation synthesis system, DSEQSYS, which uses fuzzy logic to automate the use of heuristics and this represents a hybrid between the heuristic and algorithmic approaches, (Flowers et al 1994). The system is claimed to have the advantage of being able to resolve conflicts between heuristics and, by the inclusion of the ASPEN process simulator, be able to address non ideal and non linear behaviour. Equipment sizing and process cost analysis capabilities are also included by the same means. DSEQSYS has three elements, a control programme, a fuzzy heuristic synthesis programme and a process simulator. The problem is input as a saturated liquid feed stream that is flashed to give initial physical property data. This

is then used when applying the fuzzy heuristics which generate the separations. After a separation has been selected the simulator is invoked to undertake the design. The duel synthesis and simulation routine continues until all separations have been performed or identified as forbidden. Flowers and co report on the application of DSEQSYS to five published problems where the reported results were reproduced. No possibilities for improvement seem to have been identified. Application to a new, actual design problem would be interesting to investigate as the approach shows promise for conceptual design.

Regardless of the method used there are three main problems in process synthesis that must be addressed:

(i) How to establish a representation that is sufficiently rich to include all the alternatives but that does not involve redundancy.

(ii) How to evaluate the alternatives generated to enable them to be compared.

(iii) How to locate alternatives that are improvements without requiring a full evaluation.

Reviewing the state of the art, Grossmann and Daichendt identify eight challenges in the area of process synthesis, (Grossmann and Daichendt 1996). Key is the integration of the various proposed approaches. Other areas for development are superstructures for various levels of abstraction, superstructures including non-standard unit operations, applications outside continuous processes, efficient search mechanisms for large problems, optimisation methods that are both global and multi-objective and the ability to handle rigorous models.

5.2 Material Synthesis

The task during material synthesis is to identify a material that processes the required physical properties. A brief review of work in this area is given by (Manousiouthakis and Allen 1994). The "shopping list" of required properties for a component may well be un-achievable making it necessary to concentrate on matches to those considered to be most important with flexibility allowed in others. Selecting mass separating agents for extractive separations has received a large amount of attention. Hanlon reviews tools available for formulation property

prediction and molecular simulation in the polymer field, (Hanlon 1990). Molecular simulation tools mentioned were Polygraf and Sybyl.

Material synthesis offers an opportunity to address waste minimisation right at the start of design by considering waste generating potential during materials selection.

5.3 Synthesis of Reaction Paths

Reaction path synthesis has received a considerable amount of attention over the years. The driving force behind this work has been the need for more efficient utilisation of materials and the minimisation of wastes. A review of techniques in this area is presented by Nishida and co workers, (Nishida et al 1981). Stephanopoulos identifies this area as one with a great degree of potential for revolutionising synthesis, (Stephanopoulos 1980). He also identifies those involved in reaction path synthesis as being the first to identify the potential of computer based search strategies. Algorithmic search methods have been predominant in this area. Initially it was the preserve of organic chemists focusing on the synthesis of large organic molecules. Manousiouthakis and Allen state that the important considerations during reaction path synthesis are economics, thermodynamics and kinetics, (Manousiouthakis and Allen 1994). Waste minimisation can be addressed by selecting reacting systems that minimise by product and waste generation. Inherent safety can be addressed by the careful selection of the species present to avoid hazardous properties and by the adoption of safe working conditions, (Umeda 1983). Upadhye presents an algorithm for generating sets of reactions within complex reacting systems, (Upadhye 1983). The sets of reactions generated do not reflect the actual reactions occurring but represent a means of calculating equilibrium composition. Buxton and co workers present a tool, MEIM (Methodology for Environmental Impact Minimization), which selects the most promising chemical route available in terms of minimum environmental impact, (Buxton et al 1996). The main difficulty with tools developed for this purpose is how to "rate" a reaction which has not been studied experimentally. Additionally choosing the most efficient reaction does not guarantee the most efficient process as problems could occur in raw materials or separations that out weigh the advantages gained with the reaction.

5.4 Synthesis of Reactor Systems

A considerable amount of effort has been devoted to the development of tools for the synthesis of reactor systems, some of which are discussed below, but few examples of the application of these to actual designs can be found. Many tools and techniques developed are limited to simple reactor types, PFR and CSTR, making them unrealistic. In practise conceptual reactor design, the point of application for synthesis, is the province of a few specialists backed up by R&D capabilities rather than the bulk of those undertaking design. This leads to the need to question whether reactor network synthesis tools are really necessary and useful or tools that would be dangerous in the hands of the wrong people. Is the level of interest that has been shown in their development driven by the fact that they are interesting and challenging mathematical problems or a deeply held conviction that process designers need this type of tool? Hildebrandt and Biegler discuss the importance of reaction network synthesis and contend that the performance of the reaction subsystem is key to the overall success of a design, (Hildebrandt and Biegler 1994). They discuss approaches based on both optimization of network superstructures and performance targeting with an emphasis towards techniques developed based on targeting via the attainable region concept. Disadvantages claimed for the superstructure approach are:

(i) The difficulty in establishing an adequate superstructure for general systems that can handle the inherent non-linearities.

(ii) The occurrence of local optima that may mask the overall optima.

(iii) The occurrence of non-unique optimal network structures.

Hildebrandt and Biegler strongly emphasis that reaction systems cannot be designed in isolation due to the impact on the other parts of the process and extend the attainable region concept to address this. This point of view is also held by Mehta and Kokossis who propose a methodology to incorporate multiphase reaction systems into synthesis, (Mehta and Kokossis 1996). Ishida and Tanaka discuss a system, SPEED (Structured Process Energy-Exergy flow Diagram), that uses the concept of target reactions in reaction system synthesis, (Ishida and Tanaka 1982). Donors, acceptors and sub-targets are combined to form the targets.

5.4.1 OREAN

Kokossis and Floudas looked at optimizing networks of reactors under isothermal operation with the following main assumptions, (Kokossis and Floudas 1989), and implemented the approach automatically in OREAN (Optimization of REActor Networks) :

(i) Reactors can be represented as ideal CSTR's or PFR's, with PFR's represented by a cascade of CSTR's.

(ii) The operating conditions, temperature and pressure, are fixed at nominal values for each reactor and are not optimised.

(iii) Reaction mixtures are ideal.

(iv) Homogeneous reactors are not allowed and no catalytic action can take place in any of the reactors.

These assumptions, particularly the second and fourth, place serious limitations on the usefulness of the strategy for any practical problem.

A four stage synthesis strategy is proposed with the starting point being a reaction mechanism and the kinetics that describe it and the product of the synthesis information on the number, type, volume and configuration of the reactors. Configuration information includes feeding, recycling and bypass strategies. During the first stage the various reactor types and their possible interconnections, which are embedded within a reactor network representation, are considered for applicability to the problem. Those considered applicable are then combined into a superstructure containing all the possible reaction routes. In order to reach a solution the third stage is to formulate a model of the superstructure as a MINLP problem which is run in order to obtain a solution. The objective function for the MINLP problem is a general function of the outlet composition vector and the reactor volumes.

5.4.2 RRS (Recycle Reactor Superstructure).

Achenie and Biegler propose that a superstructure based approach be adopted to reactor network synthesis, (Achenie and Biegler 1990). The superstructure containing reactors and heat exchangers is solved by an NLP with an objective function defined in terms of exit concentrations and other process variables. A high degree of flexibility is built into the superstructure which can handle recycling and

various forms of heat addition. Reactors can be linked in parallel or in series. The basic reactor module of RRS, RRM, consists of a reactor with recycle, an inlet heat exchanger, a feed stream and a recycle stream. Varying the recycle ratio between zero and infinity allows PFR and CSTR behaviour to be simulated. The option to add heat along the reactor as well as heating or cooling the inlet allows isothermal, adiabatic and non-isothermal reactions to be handled. Test cases for the strategy, based on examples from literature, are included by Achenie and Biegler. These are claimed to show that this is a viable method.

5.5 Synthesis of Separation Sequences

Separation processes constitute a significant portion of total capital investment and operating costs of a chemical plant, (Hlavácek 1978, Nishida et al 1981, Aggarwal and Floudas 1990), and consequently there has been a considerable amount of work done in the field of separation sequence synthesis. If the allowable types of separator are specified the generation of separation sequences is a relatively trivial problem, (Stephanopoulos 1980). However the selection of the optimal solution is somewhat harder. Much of this work has focused on distillation sequences and this will be discussed separately from more general developments. Early work was heuristic based but algorithmic and hybrid techniques have also been used.

Separation systems arise from the need for feed preparation and waste treatment as well as for product separation. In all cases the problem can be expressed as: given a feed stream of known conditions synthesise a process that gives the desired products for the minimum of the optimisation variable, usually cost. Independent of the criterion selected, the separation sequence resulting should not introduce waste streams that will compromise the overall plant position. This makes it necessary to consider waste generation during separation synthesis. Srinivas and El-Halwagi recognise the importance of separation system synthesis to waste reduction and propose a tool that addresses this need for membrane, pervaporation, technology, (Srinivas and El-Halwagi 1993). A state space approach is used to generate a representation that includes all the possible solutions. The problem is then solved as an MINLP to minimize total annual cost subject to environmental, technical and economic objectives.

5.5.1 Synthesis of Distillation Sequences

Much work has been devoted to the synthesis of distillation sequences. Initially work focused on sharp separations of single multi-component streams containing ideal components but has now moved on to look at more realistic problems involving nonideal multi component systems. A review of early work focusing mainly on sharp separations is given by (Nishida et al 1981) who describe the development of design heuristics for distillation processes. This development is also covered by (Nath and Motard 1981). A prototype expert system for distillation system synthesis is described by (Niida et at 1986). Two decades of work in this area are reviewed by (Westerberg 1985).

Aggarwal and Floudas look at the problem of synthesising an optimal, with respect to total annual cost, distillation sequence to separate a single multi-component stream into a number of multi-component products whilst allowing non-sharp separations, (Aggarwal and Floudas 1990). They do not take into account heat integration, assume each column preforms a simple spilt and allow the distribution of key components only in the products. A superstructure containing all options for distribution of light and heavy key components, all possible sequences and all alternatives for stream splitting, bypassing and mixing is developed along with the required cost models. The solution is reached by modelling the superstructure as a MINLP with the objective of minimising total annual cost. It is claimed that allowing non-sharp separations can result in cost savings of 10 to 30 %, even up to 70 %, over solutions using sharp separations only. This work is expanded to include heat integration between column condensers and reboilers by (Aggarwal and Floudas 1992). Here, column pressure is treated as an optimisation variable. Floudas and Anastasiadis cover the separation of several multicomponent products using distillation columns, (Floudas and Anastasiadis 1988). Here the problem is solved by modelling the superstructure of solutions as a MILP with the objective function being minimising the venture cost subject to any applicable constraints. Using the same solution method Paules and Floudas consider only sharp, non heat integrated, separations but include an investigation of design flexibility by considering the various modes of operation necessary during the synthesis, (Paules and Floudas 1988). Lu and Motard adopt a two stage process of general, high level, synthesis

based on goal targeting followed by the application of heuristics and evolutionary rules to add detail to the structure developed, (Lu and Motard 1985). Faith and Morari report on an early attempt to include heat integration into the synthesis of distillation sequences, (Faith and Morari 1979), but due to the complexity of the problem much work in this field does not include this capability. Floudas and Paules discuss a framework for the synthesis of heat integrated distillation sequences for the separation of a single multicomponent feed using sharp separations, (Floudas and Paules 1988). Column pressure is included as a variable in the MINLP formulation. The objective function is to minimise the total annual cost. Short cut methods are used to simulate the columns. Further work by Paules and Floudas included other column parameters in the optimisation to allow flexibility of the design with respect to varying feed-rates and compositions to be included in the problem, (paules and Floudas 1992). Column pressure, reflux ratio, number of trays, diameter and heat integration are included as variables to be optimised but only sharp separations can be handled. McCarthy and co workers state that genetic algorithms have been found to be more effective solvers for non-sharp separations than Newton-based methods, (McCarthy et al 1996). They propose a fully automated multi-component product synthesis tool using a genetic algorithm solution method. To provide a problem representation suitable for an algorithmic approach, product streams are regarded as outlet streams from a separation and ranked in terms of bubble point at a given pressure. A decision tree for synthesis is built from the set of transformations that the ranking describes. A recursive procedure is used to eliminate infeasible transformations.

The much more complex and realistic problem of non-ideal distillation with heat integration is discussed by (Senos Matias et al 1995). They proposed a short cut method to screen the many alternatives that arise during the synthesis of such systems. This procedure avoids a complex simulation of the column but determines all the variables necessary to calculate cost and heat requirements at the specified operating conditions. The procedure has been implemented within the CHiPS environment which is discussed further in section 5.10. Kakhu and Flower consider the synthesis of heat integrated distillation sequences using MILP, (Kakhu and Flower 1988). They found that in practically all the cases they considered, including

heat integration offered a cost advantage over non-integrated flowsheets synthesised for the same problem formulation. Douglas and co workers also discuss the synthesis of thermally integrated distillation sequences with the added complicating factor of flexibility, (Douglas et al 1991). They define a flexible process design as one that will operate feasibly for any value of the uncertain / flexible parameters and which minimises the expected annual cost of the process. This can be viewed as a two stage optimisation problem, with the outer loop optimising the items that remain fixed and the inner the operating variables that are manipulated to minimise cost. A solution algorithm based on a five stage method for exploring the solution space with uncertainty is proposed by Douglas and co workers and subjected to case study work. In comparing the effect of including uncertainty in integrated and un-integrated designs it was noted that, due to the additional heat transfer areas needed to handle uncertainty, the cost savings due to integration declined rapidly as the level of uncertainty rose. This finding should be borne in mind by those who attempt optimisation of designs during the early phases of design.

A brief review of work on non-ideal distillation is given by Malone and Doherty who point to work by Barnicki and Fair, Westerberg and co workers and themselves as being important in the development of tools in this area, (Malone and Doherty 1994). They point out that no tool available at the time represented a complete solution to separation synthesis. Malone and Doherty present a procedure combining heuristics and simplified models for use during conceptual design. The avoidance of a complete first principles model at this design phase echoes the proposals of Senos Matias and co workers, (Senos Matias et al 1995).

5.5.2 Synthesis of General Separation Sequences

Rudd and co workers were pioneers in the field of synthesis of general separation sequences with their work on the AIDES system. This was heuristic based. The size of the problem, if a truly general approach is adopted, has commonly caused the tackling of small sub problems only. Rather than concentrating on the use of models of actual unit operations, Papalexandri and Pistikopoulos present an approach where separation processes are modelled as one, or a set of, mass and heat exchange operations between two properly defined streams, (Papalexandri and Pistikopoulos 1995). To synthesise the possible alternative routes

to achieve a given separation the first step is to generate a set of streams containing all the possible intermediate streams that could appear. The alternative routes are then synthesised by considering the possible matches between the set of streams and the separation process, modelled as mentioned above. Thermodynamic based constraints are used to ensure that there are driving forces for heat and mass transfer. The separation process models use mixed-integer constraints to allow representation as combined heat and mass exchange modules. The alternatives are optimised with respect to minimization of total annualized cost as a MINLP problem. Operating costs are taken purely as utility consumptions and capital costs are sized from data contained within the system. A similar approach involving the generation of a superstructure containing all possible separation configurations that is then solved as an NLP problem is described by (Floudas 1987). Although Floudas claims the effectiveness of the approach does not rely on the separation method used, one of the basic assumptions is that only one can be used. This is stated to be "ideally" distillation casting a shadow over the claim to be a general method. Other assumptions that limit the general applicability and reality of the method are that separations are simple and involve perfect splits and that heat integration between separations is not allowable. The first of these is acknowledged as a serious limitation by Floudas. Novak and co workers also pose the general separation synthesis problem as an MINLP but propose a more general superstructure than that used by others, (Novak et al 1994). The synthesis can include one or more separator type allowing sharp and / or non-sharp separation. System topology and design parameters, including heat integration, can be optimised simultaneously, which is claimed to produce more realistic results. The approach is implemented within the PROSYN expert system set. Qian and Lien point out that the problem with all systems based on an initial superstructure from which a solution is subsequently extracted is ensuring that the initial superstructure is sufficiently rich, (Qian and Lien 1995). They propose an alternative rule based on a screening procedure to ensure that the most promising subset of alternatives is taken forward for detailed analysis.

An alternative, knowledge-based, approach is used by (Barnicki and Fair 1992). They describe a prototype knowledge-based expert system called SSAD (Separation Synthesis ADvisor) which is based around a separation synthesis

hierarchy, SSH. The SSH was developed based on interviews with experts and on knowledge contained within literature. Barnicki and Fair emphasise that SSAD is a preliminary process design tool with final design work to be carried out by a process simulation tool. This is true of all synthesis tools. SSH has four split managers: Phase, distillation, liquid and gas enabling all separation tasks, except those involving solids, to be handled. The ability to synthesise gas/vapour separation has not been dealt with in depth elsewhere. The solution strategy employed is based on an agenda management system. Splits are added to the agenda as and when a need is identified by differences between a stream and the desired products. Heuristics within the knowledge base are used to guide the selection of separation technology and the sequencing of techniques. Wahnschafft and co workers also propose a knowledge based system, SPLIT, for separation process synthesis, (Wahnschafft et al 1991). SPLIT has a blackboard architecture supporting a framework that integrates heuristic and qualitative knowledge for use during synthesis. The sum of the two knowledge types is claimed to widen the project phases that can be supported by varying the amount of information required from the user. Using a blackboard architecture also allows other tools to be integrated into the system, the inclusion of ASPEN and an optimisation programme are reported. SPLIT can be used to explore alternative solution paths but the number involved can be restricted by the application of available knowledge.

5.6 Synthesis of Heat Exchanger Networks

In reviewing the decade of work on synthesis to 1981 Nishida and co workers identify this area as the one that had been subjected to most study and hence could be regarded as the most mature, (Nishida et al 1981). This opinion is borne out by (Hlavácek 1978, Stephanopoulos 1980 and Gundersen and Naess 1988). Umeda points to the oil crisis in the early 1970s as being the driving force for much of this work, (Umeda 1983). Gundersen and Naess review state of art HENS methods and point out that all the problems have not been solved. Westerberg also reviews work in this area, (Westerberg 1989), but expands the coverage of synthesis to include work in other engineering fields. A wide range of solution techniques have been employed which Hlavácek splits into two categories: mathematical approaches and

systematic generation approaches. The pioneering work in this area was undertaken by Hohmann but HEN techniques have been systemised and made widely accepted due to the efforts of Linnhoff and co workers. Nishida and co workers discuss background work in this area. As discussed in Chapter 4 it is not possible to achieve an optimal solution to a plant design problem if heat integration is considered as a bolt on exercise after the completion of the plant design. Thus the separation of heat exchanger synthesis as a separate problem from plant synthesis is not realistic. Not withstanding this, a considerable amount of work has been done on this topic. This body of work is almost exclusively based on the pinch technology work undertaken by Linnhoff and co workers. Umeda and co workers do however propose a similar approach based on the elimination of a pinch point on a heat availability diagram that does not reference Linnhoff, (Umeda et al 1979). Two computer tools, HERP (HEat Recovery Planner) and HENS (Heat Exchanger Network Simulator) were included to aid the approach, that added integration to existing flowschemes. For given conditions in the heat exchanger network, e.g. mass flowrate, HERP provided a heat exchanger network that minimised the heat exchanger area as a function of approach temperature. HENS, was then used to evaluate the operability of the network. HERP and HENS represent two of the first reported HEN synthesis tools. The problem of HEN synthesis can be split into three parts: pre-analysis to set targets, network invention and evolution and this is the approach used by most synthesis tools.

Zhu claims that there are two serious problems when attempting to apply mathematical programming to the synthesis of heat exchanger networks, (Zhu 1995). The first is the number of small temperature or enthalpy intervals that are needed to define the shape of the composite curves leading to NLP or MINLP problems of an unmanageable size. The second is that as many NLP and MINLP solvers rely on a good starting point to reach an optimal solution the lack of such a point for HEN synthesis can cause problems. The solution proposed is to initially reduce the intervals that have to be considered by blocking together areas of the composite curves that have similar characteristics. Later crossing between the blocks is permitted to ensure an optimal solution is reached. François and Kalitventzeff propose a methodology for energy integrated HEN synthesis that takes into account

both heuristics and mathematical optimisation techniques, (François and Kalitventzeff 1989). They acknowledge the importance of factors other than cost in optimisation, citing safety, layout, flexibility and reliability. Also, via the inclusion of energy integration, HEN synthesis is coupled to the rest of the design. Trivedi and co workers adopt a two level approach, firstly generating all feasible networks that are quasi-optimal with respect to cost and than applying operability considerations, (Trivedi et al 1989). They point out that many HEN synthesis strategies have an inherent weakness in the reliability of the cost models used.

Floudas and co workers present a tool called MAGNETS (MAthematical Generation of heat exchanger NETwork Structures) for the automatic synthesis of network configurations involving possible splitting, mixing and bypassing of streams, (Floudas et al 1986). They claim that the strategy encoded in MAGNETS is unique in allowing the generation of networks that feature minimum investment cost subject to having minimum utility costs and the fewest number of units. Enthalpy is assumed to be a linear function of temperature and exchangers to be counter-current. Neither assumption is a cause for too much concern but they tend to limit realism. The method used in MAGNETS can be split into five stages:

(i) Minimum utility cost and the location of the pinch point are predicted using the LP transshipment model.

(ii) The fewest number of units at each side of the pinch is predicted using the MILP transshipment model.

(iii) A superstructure of units at each side of the pinch is derived based on the results of (ii).

(iv) Each superstructure is solved as a NLP problem with the objective of minimising investment cost.

(v) The two results are added together.

Jeżowski claims that tools such as MAGNETS that are based on MINLP solving and require considerable CPU time have a number of inherent disadvantages, (Jeżowski 1992). These are listed as the assumption of true counter-current exchangers, the assumption of constant heat capacity and the requirement for a good starting point. Jeżowski postulates that it is necessary to have designer assisted,

rather than fully automated, tools for HEN synthesis. This is implemented in the SYNHEN (SYNthesis of Heat Exchanger Networks) package where some steps are automated but some important decisions left to the user. Jeżowski implies that SYNHEN was not envisaged as a commercial tool but aimed at eastern european countries where PCs are readily available but access to sophisticated MINLP software is limited.

To increase accessibility to HEN synthesis techniques ICI developed MIDAS in the late 1980s, (Smith and Parker 1988). The aim of MIDAS was to allow non-experts to use the tool without the need for extensive training. MIDAS architecture is based on assuming a delta T_{min}, generating minimum utility requirements and estimating exchanger cost per unit area to set targets for the synthesis.

Papastrates and co workers present an interesting approach that is distinguished from other HEN synthesis tools by the inclusion of dynamic simulation capabilities, (Papastrates et al 1993). A model developed for SpeedUp is used to achieve this feature.

To overcome the inefficiency introduced by decoupling HEN synthesis from the initial stages of synthesis, Stair and Fraga propose the use of genetic algorithms to optimise the unit operating conditions of chemical process flowsheets, (Stair and Fraga 1995). The technique is implemented within the CHiPS package and allows the generated solutions to be ranked according to economic criteria. The ranking produced by considering heat integration at an early stage varies from that produced without such consideration.

Sandoval and Zhu proposed a three phase decomposition of the simultaneous synthesis of heat integrated distillation sequences, (Sandoval and Zhu 1996). In the first phase, separation sequence screening, the focus is on separation sequence and operating conditions with a trade off between HEN capital costs and energy costs. Secondly the initial HEN is synthesised as the solution to a MILP problem. Finally the HEN topology is optimised. A two stage decomposition is proposed by (Muraki and Hayakawa 1987). Firstly the distillation sequences are synthesised, using heuristic rules, and these are then optimised, with respect to minimum total annual cost, by the introduction of energy integration. The best alternative is then selected. Rather than decompose the HEN synthesis problem, as most workers do, Ciric and

Floudas propose an approach where a single MINLP optimisation problem is posed, (Ciric and Floudas 1991). They claim that each element of the decomposition approach adds uncertainty as to the optimality of the network obtained. In their approach the MINLP is solved simultaneously for utility consumption levels, process stream matches and optimal network configurations making it unnecessary to make any assumptions of pinch points, minimum utility consumption levels or minimum number of units.

Chen and co workers proposed an expert system for the synthesis of heat exchanger networks, (Chen et al 1989). The system described, SPHEN, was designed to mirror the synthesis strategy adopted by an engineer. Firstly SPHEN identifies the presence of pinch points and then uses a heuristic method to construct a network that fulfils the requirements of minimum utility cost and the fewest number of units. These units are then matched to exchanger types and simulation undertaken. The user views the results of the simulation and undertakes iterations until a satisfactory network is obtained.

5.7 Control System Synthesis

Nishida and co workers point out that control theory supposes that the measured and manipulated variables have been preselected, (Nishida et al 1981), and thus specifying the control structure. Early attempts to provide assistance in selecting the control structure are then discussed. The first step must always be to determine the control objectives followed by the selection of controlled variables, selection of measurements, selection of manipulated variables and the final step is to choose how to connect the measured and manipulated variables. Stephanopoulos briefly discusses the objectives of control system synthesis, (Stephanopoulos 1980). These are identified as the variables to be measured to monitor the process, the variables to be manipulated to control the process and the relationship between the measured and manipulated variables. Niida and co workers discuss a prototype expert system for the synthesis of distillation control systems, (Niida et al 1986).

In a review article exploring a decade's work on synthesis of control structures Morari and Perkins concentrate on methods of evaluating control structures so that they may be compared, (Morari and Perkins 1994). The split is between

evaluations based on steady-state, linear dynamic and nonlinear dynamic models. Morari and Perkins point out that little work has been done on synthesis in this field and question the likelihood of useful synthesis tools in this area appearing in the near future. Problems in evaluation are highlighted as being the main reason for this pessimism. Mohideen and co workers present a more sweeping method of tackling control system synthesis in parallel with process structure synthesis, (Mohideen et al 1996). Dynamic modelling is used for the structure with control system design incorporated into the optimization problem. Huang and Fan propose an approach for the inclusion of controllability into the synthesis stage of process design, (Huang and Fan 1992). Whilst not a synthesis of a control system structure this allows operability to be addressed at a stage where fundamental change can be made.

5.8 Mass Exchanger Network Synthesis

Mass exchanger network (MEN) synthesis was developed in response to concerns over waste minimisation. A review of the field is given by (Manousiouthakis and Allen 1994). The synthesis task can be defined as: "Given a set of rich streams and a set of lean streams, synthesise a network of mass exchange units that can transfer certain species from the rich streams to the lean streams at minimum venture cost". A mass exchange unit is any counter current mass transfer operation and the MEN synthesis task is to identify the type, number, size and interconnection of these units that optimise mass transfer. The approach proposed is somewhat similar to HEN synthesis. Papalexandri and co workers present a modification of the basic MEN approach that does not require the problem to be decomposed around a pinch, (Papalexandri et al 1994). The synthesis problem is formulated as a MINLP which is solved by optimising network operating and investment costs simultaneously.

5.9 Whole Plant Synthesis

Rather than optimise a series of sub-problems the best way forward is to consider the whole synthesis problem together. This has the potential to add complexity and increase computational times significantly.

Early entrants in the field of computer-aided whole plant synthesis were

AIDES, by Rudd and co workers, and BALTAZAR, by Mahalec and Motard. AIDES used heuristic procedure and considered all streams in parallel. Weighted heuristics were used to rank alternatives, (Mahalec and Motard 1977). BALTAZAR used evolutionary search techniques and considered each destination stream in turn whilst attempting to eliminate property differences, (Nishida et al 1981). Neither AIDES or BALTAZAR calculated sizes or costs. Tackling the whole problem rather than decomposing it into the above sub problems adds complexity and limits the ability to address all alternatives in a comprehensive way. Umeda argues that whole plant synthesis would not be solved even if all the other sub-problems were solved, (Umeda 1983). This represents the most difficult synthesis problem. The Douglas hierarchical approach to design discussed in Chapter 4 is a whole plant synthesis method. The implementation of this as a computer based design tool is discussed by (Kirkwood et al 1988).

Early work on whole plant synthesis is reported by Lu and Motard who propose a heuristic-evolutionary approach, (Lu and Motard 1985). They define the general flowsheet synthesis problem as developing a process flowsheet that converts available raw materials into desired products in the most economical way. To represent the problem two stream matrices are used, in which streams are expressed in terms of species, quantity, enthalpy, pressure and other parameters. The differences between the goal matrix, representing the desired products, and the source matrix, representing raw materials and uncommitted intermediate streams, are used as the keys for the application of operators. This action moves the design from the source to the goal state. Only basic operators: reactor, mixer, separator, pressure changer and enthalpy changer, were included in the work described. Lu and Motard adopted a two level hierarchical structure, which had been implemented with respect to separation only, to tackle the synthesis problem. At the top level rule based synthesis obtained the process scheme and at the second level more equipment detail was added to allow costing to take place. An indirect cost criterion is used at the top level, where insufficient detail is available for full costing, to control the generation of alternatives. Schemes are generated by applying operators to groups of consolidated sources in order to achieve goals. More than one goal may be realised from one such application, a process referred to as goal lumping. The higher the

degree of lumping the lower the number of operators involved in problem solving. Successive linear programming is the basis for carrying out this solution strategy terminating when all goals have been satisfied. Heuristic and evolutionary rules, applied in a hierarchical way, are used to add definition during stage two. Chan and Prince also propose a heuristic approach, (Chan and Prince 1989). In their approach the flowsheet is built up unit by unit using heuristics to eliminate those alternatives that are unlikely to be optimal. Optimisation occurs at each step. The basis of the approach is to consider each stream at a time until destinations have been assigned in all cases. Recycle of streams between units is included but it is not clear how much backtracking is associated with a decision to recycle. Six possible flowsheet modifications are available:

(i) Recycle. To assign a stream to an existing unit.

(ii) Join. To combine two unassigned streams and pass them to a new unit.

(iii) Newcell. To process the stream in an additional unit.

(iv) Remove. To remove a unit and assign the feed(s) as a system output.

(v) Return. To remove a unit and assign the feed(s) to units who's feed they exhibit the closest match.

(vi) Offspec. To remove a unit and allow the feed(s) to be system outputs, if of sufficient specification, or to use them as feeds to other units.

The use of the system for synthesising flotation separation systems is discussed.

Kokossis and Floudas report on work that moves towards whole plant synthesis by considering problems with reactor and separator systems linked by recycle streams, (Kokossis and Floudas 1991). The system proposed is based on a general superstructure containing all configurations of the reactor-separator-recycle system. This is then solved as a MINLP. The realism of the method is called into question by some of the base assumptions used. These are:

(i) All separators are considered to be simple distillation columns with sharp splits.

(ii) Reactors are CSTRs, with PFRs approximated as equal volume CSTRs.

(iii) The thermodynamic state of streams is assumed to be known.

(iv) Unit operating conditions are fixed at nominal values and not optimised.

(v) No heat integration takes place.

The final two are the most restrictive and this is acknowledged by Kokossis and Floudas. PROCESS was used to obtain the parameters required by the cost models used during optimisation. Omtveit and co workers also propose the use of decomposition to tackle large synthesis tasks, including reactors, separators and recycle, (Omtveit et al 1993). Details of the basic assumptions used and models included are not given. A two level decomposition is proposed. At the top level a mathematical model of the flowsheet is used to generate mass balances that are used in the search for an optimal combination of reaction conversion and purge fraction. A basic economic analysis based on stream costs / values is also carried out. At the lower level the reactor system and heat integrated separation are synthesised as separate MIP models. Costs are returned to the upper level for use in solving the optimisation problem.

Diwekar and co workers report on an extension of the ASPEN simulator to add a process synthesis capability, (Diwekar et al 1992a). This was specifically aimed at selecting the optimum from three alternatives for integrated gasification combined cycles (IGCC) with special consideration of environmental impact. The basic models of the alternatives were developed by the US Department of Energy with the MINLP problem necessary for the selection of the optimal being added by Diwekar and co workers. This application was one of the first to add process synthesis capabilities to ASPEN. A more general description of the approach and the algorithms used is given by (Diwekar et al 1992b). Kravanja and Grossmann propose a procedure based on a general superstructure of flowsheets that allows simultaneous optimization and heat integration, (Kravanja and Grossmann 1990). This involves the solution of MINLP problems. The strategy proposed is implemented within the PROSYN computer package. PROSYN uses a heuristic branch-and-bound technique to generate the most promising process alternatives. A suite of expert systems, termed a knowledge integrating system, are used to handle the detailed engineering knowledge required, (Schembecker et al 1994b). A link to ASPEN is used to simulate unit operations and calculate economic data.

Crowe and co workers report the development of an expert system for whole plant process synthesis that gave results similar to those previously published for four diverse problems, (Crowe et al 1992). Whilst these could not be guaranteed to be optimal they appeared to be reasonable. The expert system developed did not include equipment sizing, costing or economic analysis routines as it was concluded that all complex issues were best left to the engineer and separate analysis software. Given a list of product streams or goals, the stoichiometry and extent of reactions and, optionally, a list of potential raw materials and / or a partial existing flowsheet the system will generate a flowsheet. This will represent a reasonable way of achieving the goals whilst minimising mass flows through separators, minimising the total number of separators and maximising the recycle structure. The ability to include an existing flowsheet in the problem allows retrofitting to be addressed. Crowe and co workers used top level, synthesis and garbage rules within the expert system. Top level rules control the operation of the system. Synthesis rules add or modify the flowsheet structure to reach a goal. Garbage rules check for consistency and redundancy. For problems with multiple goals recycle is necessary to achieve a full solution.

Kirkwood and co workers also adopted an expert system approach to flowsheet synthesis during the development of PIP (Process Invention Procedure), (Kirkwood et al 1988). This is based on the Douglas hierarchical model discussed in Chapter 4 hence the solution strategy employed by PIP is quite different to that used by Crowe and co workers. Work to debug the PIP code was still ongoing in 1992, (Rajagopal et al 1992). Both qualitative knowledge, such as heuristics, and quantitative knowledge, such as unit operation models, are utilised in PIP. Such combinations of knowledge types, with their separate knowledge bases, are seen by Kirkwood and co workers to represent the future of expert systems in process engineering design. Heuristics are used for high level activities such as identification of alternatives and selection of unit operations. At lower levels in the hierarchy quantitative models are used to calculate flows, sizes and costs. This represents a much more sweeping approach than that proposed by Crowe and co workers with little left to the discretion of the engineer. Kirkwood and co workers argue that sizing and costing routines are essential to allow optimisation to be carried out. The

aim of PIP is stated as to improve the productivity of the process engineer during the initial phase of design with a time of one hour claimed to be all that is required to produce a design that would take two days using conventional methods. PIP requires definition of the required product, feed-streams, reactions and physical properties to carry out a synthesis. As with the manual Douglas method PIP generates a base case design and backtracks to look at alternatives if this proves to be profitable. If the base case proves to be unprofitable at any level alternatives are evaluated immediately to determine if any profitable pathways exist. Energy integration is considered at the lowest level only. The limitations of the methodology are discussed in Chapter 4. To validate the heuristics employed PIP was tested against base case flowsheets and acceptable results were claimed by Kirkwood and co workers in all cases, although non-ideal separations could not be handled. Raman and Grossmann argue that a system using both qualitative and quantitative knowledge is essential for a robust approach to synthesis, (Raman and Grossmann 1992). A system based solely on qualitative knowledge requires a large knowledge base and they claim this cannot produce optimal designs. Using quantitative model based knowledge allows a rigorous solution including optimization to be produced but there are often limits on the problem size that can be handled. Raman and Grossmann propose two possible means of including quantitative knowledge in synthesis, at the level of model formulation or at the level of the MINLP optimisation algorithm. Both approaches are claimed to be successful. Engelmann and co workers propose a system of distributed expert systems, arranged in a hierarchy of increasing detail, for use in synthesis, (Engelmann et al 1989). At the top level a manager co-ordinates work and calls process specialists as necessary. These in turn can call service specialists to provide detailed information.

Petrides and co workers address the synthesis and design of waste treatment plants using three knowledge bases within a KBES, (Petrides et al 1994). The system proposed, EnviroCAD, takes as input the waste streams generated by a plant. These are analyzed and alternative schemes based on recovery, recycle, treatment and disposal generated. Included with EnviroCAD are simulation and costing capabilities to ensure that ranking of alternatives is possible. This is far from a general synthesis tool but with the addition of the appropriate knowledge bases and models the

approach could be extended.

5.10 CHiPS

CHiPS is a process synthesis package developed by the ECOSSE group at Edinburgh University for the automatic generation of economically efficient and environmentally acceptable processes. The aim of a synthesis package is not to provide a complete solution to a problem but to give the process engineer a suitable starting solution to a problem, (Fraga and McKinnon 1993). Using a synthesis tool during the early stages of design should help the engineer explore an increased number of alternative solutions within, hopefully, a shorter time scale. It is these two apparently conflicting goals that CHiPS aims to address. CHiPS uses parallel programming techniques with branch and bound searching of the superstructure during solution generation. Dynamic programming techniques allow the efficient re-use of solutions as appropriate and the generation of multiple, near optimal, solutions, (Fraga 1995b). As an outcome the user is presented with the number of best solutions requested, these can then be analyzed using more stringent techniques to give more confidence in the results. This two level strategy, when fully implemented, will require the use of simple models during the initial exploration phase followed by rigorous, computationally intensive, models for fine tuning. As an approach to optimisation dynamic programming produces a solution which is composed of the solutions to one or more sub-problems. The sub-problems being derived deterministically from the problem without the need for the user to take any action. Each sub-problem consists of a stream, virtual heat links for the incorporation of HEN synthesis and qualifiers to set conditions on the solution. The inclusion of energy content as a stream attribute within CHiPS allows heat, as well as mass, balancing to take place. Additionally, the possibility of energy mismatches between units is avoided. Details of CHiPS methodology are given by (Fraga 1995b). Heat integrated flowsheets including non-sharp separation, reaction and recycle can be handled but integration can be disabled if desired.

5.10.1 Description of CHiPS Functionality.

The interface through which the user communicates with CHiPS is described by (Fraga 1995a). This interface is one of four layers contained within the system,

the others being optimization modules, unit models and the support library. The unit model interface (UMI) and other parts of the system that are of interest to unit model designers are contained within the support library and would not be of interest to the average user. However CHiPS is set-up to allow ease of addition of models if those required by the user are not present. To this end UMI is a Fortran and C compatible interface. Initially the models incorporated were:

(i) Sharp and non-sharp distillation columns based on the Fenske-Underwood-Gilliland method.

(ii) Sharp and non-sharp isothermal absorber based on the Kremer equation.

(iii) A sharp and non-sharp isothermal, adiabatic flash model, a preset recovery flash model and a multi-purpose flash model.

(iv) A well mixed ideal fixed conversion reactor and an ideal plug flow reactor for simple irreversible reactions.

Fraga describes later distillation, reactor and mixer models. (Fraga 1995b). Here the distillation model is based on the Fenske-Underwood-Eduljee equations and the separations assumed to be semi-sharp.

All CHiPS commands are in lower case letters and there is an ability to add comments into input files by prefixing a line with a % or a #. Commands available within CHiPS fall into four areas: problem specification, optional settings, output display and the help system. Once a command is entered CHiPS enters a command submode that contains specific help and must be terminated using "end" or "quit". The command areas are discussed in turn below:

5.10.1.1 Problem Definition.

A CHiPS problem is defined by a list of components, the feed stream, a list of acceptable products and a list of units allowed in the flowsheet. Using the input feed stream, defined using the "feed" command, and the list of allowed units CHiPS traverses the possible flowsheets to find the optimal one which satisfies the specified products. Within the feed command submode the components in the feed, pressure, temperature and state may be specified by the user. Setting different levels allows the effect of operating conditions on the overall process to be investigated. The "components" command is used to specify the list of components known to the

system. In the components submode the components and their associated physical properties are specified. Unit types allowable in the synthesis are specified using the "use" command. Finally the list of acceptable products is specified using the "products" command. Input to CHiPS can be interactive or via a pre-prepared input file. In addition to the ability to interact via text commands CHiPS has been implemented within the épée environment, (Fraga and McKinnon 1993).

5.10.1.2 Optional Settings.

Once the four items discussed in section 5.10.1.1 have been defined CHiPS can attempt to find a relevant process flowsheet without the user having to provide any more information. However if there is more specific information available to guide the synthesis this can be input by the user as alternative values of the default settings for a whole range of variables. A list of general user definable variables is contained within the CHiPS user's manual. Examples are the key component recovery, minimum utility temperature approach and the number of best solutions to be presented to the user. A strict format must be adhered to when setting variables to ensure that they are recognised by the system. The protocols used include the absence of spaces between variable name, equals sign and the value and the use of colons to specify range limits and number of steps. In practise the protocols were found to be much more flexible than indicated. Additionally some of the internal variables for CHiPS models can be altered by the user through the UMI. Examples are tray efficiency and recoveries for a distillation column.

5.10.1.3 Output Display.

A design generated by CHiPS can be viewed in either textual form or graphically. The "print" and "plot" commands respectively are used. The selection of the N best flow schemes to present to the user is on an economic basis. This mode of operation allows the user to retain control of the designs that are selected for further analysis. If only a single "optimal" solution based on assumptions necessary during the early stages of design were presented to the user it is highly unlikely that this would prove to be the overall optimal solution. If a high value of N is used the amount of memory required to store the results is high and there is a risk that the user will be unable to adequately utilise all the information presented. A balance has to be struck between the need to explore alternatives and the need to

prevent the user from becoming bogged down by an embarrassment of design information.

5.10.1.4 Help System.

Online help is included within the user interface, giving a list of commands that are understood by CHiPS and detailed information on any specified command. This information is accessed by typing "help" followed by the command name. This information is not repeated in the user's manual, (Fraga 1995a), as it is assumed that users will have CHiPS available when tackling a problem.

5.10.1.5 CHiPS Implementation Issues

CHiPS can be used in a number of ways, for the synthesis of whole plants or separation sequences only, for synthesis including heat integration or without it. The mode of use selected by the user is dependant on the design stage reached. The most complex calculation performed by CHiPS is the synthesis of a heat integrated whole process. The inclusion of heat integration within synthesis, rather than as an add-on after the flowsheet structure has been fixed, is a key issue for CHiPS, (Fraga and McKinnon 1993). The implementation of heat integrated synthesis adopted builds on work undertaken by (Dhallu and Jones 1988). Of the alterations to the basic methodology the most fundamental is the decoupling of the design of unit operations and the associated heat exchangers. This allows efficient use of basic unit models and simplifies the task of writing new models. Fraga and McKinnon concede that the heat integrated structures initially generated by CHiPS may not be optimal but, after refinement, they are better than those generated without the simultaneous consideration of heat integration during the initial stages of design. This option was not explored during testing.

As CHiPS does not decouple the structural and HEN synthesis, using the representation of virtual heat links express heat fluxes instead, it is computationally intensive. To address this Fraga and McKinnon look at the implementation of CHiPS on a cluster of unix workstations, as these are more common than parallel computers, (Fraga and McKinnon 1995). The strategy used is claimed to have minimum impact on other workstation users whilst giving considerable speed-up for CHiPS over a sequential implementation. Recognising that the majority of users will not have access to advanced computer architectures CHiPS is designed to run on a

minimum of a Unix workstation or PC compatible with at least 8 Mb of memory.

5.10.2 Comments on CHiPS Usage

It was not possible to use the HF acid case study whilst running CHiPS as the models available were inadequate for the unit operations associated with a system including solids. The ability of the reactor models to handle only a single reaction and the inclusion of only ideal distillation models also represented severe restrictions. Work to include non-ideal distillation was ongoing at the time of the study. An alternative study using the MEK from 2-Butanol process was therefore used. A worked chemical engineering design solution based on this process is given by (Austin and Jeffreys 1979) making a significant amount of background information available. Data extracted from this source included product component levels, distillation column parameters and reaction rate equations. Having a completed design available as an information source does not reflect the situation that would be available in most synthesis situations. Having a high level of pre-knowledge can cause the user to pre-judge the outcome of synthesis and influence the exploration that is undertaken. There is a balance to be struck between innovative synthesis and the use of prior knowledge, captured as heuristics, to guide a design.

Once a few bugs with system set-up had been ironed out CHiPS ran. The combination of the User's Manual and on-screen help was not sufficient to permit the problem to be set-up and run without any further assistance from the developers. Initial attempts at a run, using the interactive inputting mode, were completely unsuccessful as the on-screen help was not of sufficient detail to guide a novice user. The prime reason for failure was confusion over the set-up of the reactor rate equations and the need to include mixer units. At various points during the attempted input preparation seemingly helpful error messages where generated by CHiPS referring to the help system for further details, but all that was contained within help was a repeat of the error message. Subsequently use was made of a pre-prepared, via a text editor, input file as described in the user manual but here problems were encountered because on-screen help was, obviously, not available and the user manual does not reproduce the necessary information. Some minor conflicts between the two help sources were also discovered. Most seriously, without access to on-screen help, it is not possible to obtain details of the available models, the

settings within these models and the default values. To have this information to hand whilst preparing the input file it had to be copied down from within CHiPS. The default values supplied by CHiPS should be realistic and in most cases no problems were uncovered. Worryingly the default process conditions for feed streams had been set at -1.0 K, a physical impossibility, and -1 atm, a perfect vacuum. To encourage confidence in the values of other default settings these should be set at much more realistic values, say normal, 273 K and 1 atm, or standard, 288 K and 1 atm, conditions. Also related to feed definition, CHiPS should be altered to allow the inclusion of multiple feed streams of varying composition.

Neither of the two alternative inputting modes available to the user in CHiPS, interactive and input file, are very user friendly. The interactive mode required the user to do most of the work without prompting or information on the required data. A GUI based system would be necessary to make user interaction in-line with other currently available tools and this was under development for épée at the time of testing. Today users would not accept the need to remember input protocols in a commercial tool. Such attributes may be considered window dressing to be added when the tool is being prepared for commercial use but are essential if tools are ever to make the leap from research applications into general usage. Figure 1 shows an example of a CHiPS input file.

Physical properties can be specified by the user via a physical property file containing values of the critical parameters to be utilised by the programme during calculations or by the use of a PPDS file. In either case the user should not be forced to specify a file for each combination of components but should specify a single file containing all possible components, with associated methods, from which the programme picks those to use.

CHiPS allowed the same component to be added more than once to the feed composition without picking up any conflict of names. Multiple instances would lead to the possibility of alterations in default settings not being carried forward into synthesis and should be avoided. Using the interactive mode it was difficult to make alterations to the feed component list once it had been entered. The ability to add and delete components, as per the products list, should be included.

At the time of the test it was not possible to add costs to CHiPS feed streams

but values could be placed on products. This makes it difficult to run meaningful comparisons of a single process with several possible feedstocks, such as the HF acid process. Also in the cost area CHiPS uses utility prices expressed as Cost / GJ. This is not intuitive to designers, who tend to work in terms of Cost / Flow, and can lead to unrealistic results based on a zero temperature difference, indicating an infinite flow. This basis can easily be changed and should be to avoid confusion.

Setting the list of allowable units with the "use" command was straight forward with a reasonable amount of help for the novice user on-line. A list of unit types available could be brought up with a very brief description. The following were available for use during the test:

(i) dist. Ideal distillation unit based on F-U-G.

(ii) condist. Ideal distillation with pre-heater / cooler.

(iii) comp. Heat exchanger for pre-heating or pre-cooling a stream.

(iv) reactor1, 2, 3 and 4. Well mixed isothermal reactor unit.

(v) mixer1, 2, 3 and 4. Mixer unit for feeds and recycles.

(vi) 2cs. A zero cost "magic" separator for new technology studies.

This list does not agree with the claims of model availability expressed in (Fraga 1995a). The obvious complete gap is any form of pressure changing device. The different instances of the reactor and mixer models included contained the same default value sets and had been included to allow more than one reactor, with different default settings, to be included within a scheme. Such an approach is potentially very wasteful of time and space, particularly if carried through to items that are likely to occur frequently within a flowscheme, eg distillation columns. A more satisfactory approach would be to have a single version of each model within CHiPS which can be called up by the user as many times as required for a given problem, with parameters set as necessary. For each of the models present the default settings where clearly stated and explained within CHiPS and a help page available giving background information. Typing "use dist", for example, adds the distillation model to the list of units to be considered without giving the user the option of accepting the default settings or inputting alternative values. A simple yes / no response to "Do you wish to alter the default settings?" leading, as appropriate,

to a sub-menu to permit changes to be made would ensure that the user has to, at least transiently, consider the applicability of the default settings to the problem being considered. With the exception of 2cs all available models were considered for use during the test case. No major problems were uncovered but the need to supply components to the mixer model and information on recycle flows were considered anomalies that should have been dealt with automatically by the programme. To achieve success in running the test case the most helpful element was found to be an example of a previously run input file.

The inclusion of the "nouse all" command in the CHiPS input file was necessary to ensure that information from previous runs had been cleared from the system. This should be automatically kicked-in by the system when a new run is commenced.

The alternatives generated during the initial run can only be subsequently refined, for example, by the application of further HEN synthesis. This can only be done for one alternative at a time which is rather cumbersome for anything other than a small number. Any improvements that result from these refinements are not reflected in the list of N best solutions which remains as initially generated, raising the possibility of a solution closer to optimal being overlooked.

5.10.3 Subsequent Developments

Due to difficulties encountered with attempting to run the HF Acid case study during testing, further work was subsequently undertaken to develop the necessary models and include the required physical properties, (Laing and Fraga 1996). Three unit models: an acid blender, kiln reactor and absorption column were included. Short cut methods within CHiPS were used to supply properties for those components not supported by PPDS. Laing and Fraga focused on the Buss process for HF production therefore the models developed are rather specific, taking Fluorspar and a mixture of Oleum and 98 % H_2SO_4 as feedstocks. This approach limits the exploration that can be expected and does not tie-in with the breadth rather than depth approach used during the work described there. Focusing on one particular route limits the innovative aspects of a synthesis tool. The case study work takes a staged, hierarchical, approach with tightening of waste stream specifications to meet environmental constraints as the design progressed.

5.11 Developments Required.

To fully utilise the creative possibilities promised by synthesis tools the aim must be to develop tools that become as widely accepted and used as simulation tools currently are. The list given below identifies the attributes of a synthesis tool required to achieve this and reviews where CHiPS stands on each of the issues.

5.11.1 User friendly.

The user should not have to be a computer programmer in order to obtain meaningful results to real problems. Most users now consider the use of GUI technology for communication with a programme to be essential. On screen help facilities are generally viewed in the same light. The aim should be that a user should not have to go through an extensive learning curve at each use of the tool. CHiPS does include on-screen help facilities which are more extensive than the user documentation but even these are not adequate to support the novice user. At the time of testing the GUI for épée was still under development and the available forms of inputting were not user friendly. The use of input files has advantages when it comes to running several cases using some common elements as these can be cut and pasted together as necessary. During testing the use of input files was the preferred means of inputting and the required format was found to be sufficiently forgiving of misplaced commas etc to be robust.

The mode of presenting run results to the user is equally important as the mode of inputting. If the results are presented in such a way that they become difficult to interpret and utilise then the user will be unable to extract the maximum benefit from the tool. CHiPS can present the user with a rather crude plot of each of the alternatives requested which shows the reactors and separators but not the heat exchanger network. Results would be better presented in a style closer to a PFD with a table containing supplementary data, such as costs, at the bottom of the chart. Figures 2 and 3 show none graphical CHiPS output including the various levels of detail available.

5.11.2 Extensive range of models available.

As the majority of users will have neither the time nor the skill to add tailor made models, a large database of models, similar to those contained within simulation tools, should be available. This is particularly important within large

organisations where the requirement of quality control to have an auditable trail for the design means that all methods used have to be easily verifiable. In such situations if a large number of users were each adding new models to tools they were using the ability to adequately check the work undertaken would be seriously compromised. Model development is best left to a small group of experts who would also be responsible for method testing and approval prior to release for general use.

5.11.3 Ability to model "real" problems.

Limitations on reaction types, solid phases etc. that can be handled need to be removed. Moves in this direction are being made for CHiPS, (Laing and Fraga 1996), but this is a process that will take a number of years and be dependant on the industry sectors who embrace the use of the tool.

5.11.4 Range of problem specification.

A synthesis tool should avoid being too prescriptive over the form in which the problem must be specified by the user. The various starting points for design discussed in Chapter 1 need to be supported. Exploration of products feasible from known reactants or reactants to produce desired products must be equally well supported.

5.11.5 Choice of best solutions.

The "N" best solutions presented to the user are selected by CHiPS based on an economic ranking. This ranking is determined using cost models embedded within the programme, the basis of which is not obvious to the user. Unless the basis is clearly stated there will be a question mark in the users mind over the validity of the ranking. Such a situation would adversely affect the wide scale adoption of CHiPS as a tool for the early phases of design. As with virtually all of the parameters involved in a CHiPS model the user can supply alternative cost correlations but these must be carefully checked to ensure that they have a consistent time and monetary unit basis. CHiPS uses the USA Marshall and Swift Index for updating costs, whilst the Process Engineering Index is more extensively used in the UK, the index used is relatively unimportant.

As discussed in Chapter 4 economics cannot be taken as the only factor to be considered when deciding between design alternatives. If it is not feasible for multiple factors to be used to produce a single list of best solutions within CHiPS

then it will be necessary to produce a number of such lists each based on a different criterion. Whilst such an approach is not mathematically elegant it does allow the user a high level of control over the selection of the features that are important to the design under consideration. Moving to a single, multiple factor index would effectively remove the user from the decision process and, by giving the programme many variables to optimise co-incidently, would result in long run times. The multiple rankings approach is to be adopted by CHiPS in future work. As a first pass at this work environmental impact and safety should be included.

5.11.6 Ability to support high level design.

During the very earliest phase of design, when little is known about the process, it is difficult for the user to make a meaningful selection of unit operation based models to be used during the synthesis. What is required are effectively "black boxes" to look for the need for reactors, phase changers and separators without the need to go into details of models of any items of equipment. This is analogous to early attempts at synthesis that focused on the elimination of phase and chemical species and physical property differences. To use such a system the user would simply input information on the components present in the feed, desired products and estimated conditions of the two streams. Given the short execution time of such a system a relatively large number of runs could be undertaken by the user as an aid to exploration. Even the first, simplified model, level of the proposed CHiPS strategy includes a greater level of detail than envisaged.

5.12 Conclusions

The limited range of models available in CHiPS currently limits the utility of the tool at the time of testing. Whilst problems were experienced with the quality of help available CHiPS did produce successful results within a reasonable time frame. Improved, primarily graphical, means of presenting the results to the user are required if CHiPS is to be adopted on a wide scale. Also critical to success is an enhanced help system. To fully support the design process a synthesis tool needs to be available to the user from the earliest phases of design and therefore contain models of increasing complexity. CHiPS is starting to move in this direction.

FIGURE 1

```
% This is an example for the use of CHIPS using the MEK from 2-Butanol process.
% The input file has been created using textedit, using an example input file
% created by Eric and the user manual as the basis. Also on-line help consulted
% as necessary.
%
% Need to reset the models.
nouse all
%
% Reaction 2Butanol ----> MEK  +  Hydrogen
% Defines component properties
components
        comp 2Butanol    flow=17.5 code=172
        comp MEK         flow=17.5 code=71
        comp Hydrogen    flow=17.5 code=38
end components
%
% Defines the components in the feed
feed
        comp 2Butanol    temp=293
end feed
%
% Having defined the components and the feed what remains is to define the
% products and the models that can be used. It may also be necessary to look at
% adjusting settings on the models.
%
% Defines the reactor
use reactor1
set reactor1 conv=( 0.90 )
set reactor1 rur=true
set reactor1 nc=3
set reactor1 temp=723
set reactor1 comps=( 2Butanol MEK Hydrogen )
set reactor1 stoich=( -1 1 1 )
set reactor1 minflow=15
set reactor1 maxflow=100
set reactor1 keycomp=2Butanol
set reactor1 k="c c /( 1 -  c c )"
show reactor1
%
% Defines the distillation model to be used for product separation.
use dist
set dist toprec=( 0.99 )
set dist botrec=( 0.99 )
set dist te=0.38
set dist rr=1.28
show dist
%
% Now need to define the products
products
        add
                comp MEK xf>0.99 flow>15
                comp 2Butanol flow<0.5
        end
        add     comp Hydrogen flow>15
                comp MEK flow<0.1
                comp 2Butanol flow<0.1
        end
        list
end
%
% Will run initially without heat integration, i.e. no need to set-up heat
% links. Not sure that I have fully understood the use of these.
%
set pp_ppds=true
set flowtolerance=10
% Starts the design
%
design
%
% Shows the solution in text form.
%
print verbose
```

FIGURE 2

```
Component 2Butanol added with ID 0, label A, base flow 17.5 kmol/hr
Component MEK added with ID 1, label B, base flow 17.5 kmol/hr
Component Hydrogen added with ID 2, label C, base flow 17.5 kmol/hr
temp: not a valid keyword.
Feed (1 A ) defined.  Use 'show feed' to display.
CHIPS Warning: conv expects '( a ... )' with 8 entries but 1 found.
CHIPS Warning: comps expects '( a ... )' with 16 entries but 3 found.
CHIPS Warning: stoich expects '( a ... )' with 16 entries but 3 found.
Using unit 'reactor1': Well mixed isothermal reactor unit
                nc (Number of special components) : 3
              conv (Conversion rates) : 0.9 0 0 0 0 0 0 0
              temp (Reactor temperature) : 723
             comps (Components) : ( 2Butanol MEK Hydrogen                )
       conceptual (Level of design) : false
            excess (Excess of component required) : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0
           minflow (Minimum key flow) : 15
           recfrac (Recycle Fraction) : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
            stoich (Stoichiometry) : -1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0
        instrcost (Instrumentation cost) : 4000
           makeup (Amount of make-up allowed) : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0
           keycomp (Key component) : 2Butanol
                 k (Rate constant (expression in x, the conversion)) : c c /(
1 -  c c )
          ldratio (Length/Diameter ratio) : 6
          maxflow (Maximum input reactant flow) : 100
              rur (Recycle Unused Reactants?) : true
       limitequil (Reaction is limited by equilibrium) : true
             cost (Cost function) : 1917 D^1.066
CHIPS Warning: toprec expects '( a ... )' with 4 entries but 1 found.
CHIPS Warning: botrec expects '( a ... )' with 4 entries but 1 found.
Using unit 'dist': Ideal Distillation Unit based on FUG
                rr (minimum reflux ratio) : 1.20
                pm (pressure matching) : true
           toprec (tops recoveries) : 0.99 0 0 0
           botrec (bottoms recoveries) : 0.99 0 0 0
            stats (statistics) : 0 0 0 0
               te (tray efficiency) : 0.38
             name (a test for string vars) : Minerva
           reftemp (Enthalpy reference temperature) : -1
              asr (Allow stripping/rectifying column designs) : true
          msindex (M&S Cost Index (280 for 1968)) : 288.4
          colcost (Column Cost function) : (1+(P>3.4)(0.0147(P-3.4)))(4.23 ms
index/280.0 7620 D (H/12.2)^0.68)
         traycost (Trays Cost function) : 0.61 $ msindex/280 111.41 (D/1.22)^
1.9
        maintcost (Maintenance Cost function) : M ( colcost + instrcost + tra
ycost )
        instrcost (Instrumentation Cost function) : 4000
             cost (Cost per year function) : TAX maintcost + (colcost + trayc
ost + instrcost)/     LIFE
          eduljee (Use Eduljee correlation instead of Gilliland) : false
       conceptual (conceptual) : false
No products yet defined.
 1.     [MEK, xf > 0.99, Flow > 15 kmol/hr, Value 0]
        [2Butanol, xf > 0.00, Flow < 0.5 kmol/hr, Value 0]
 2.     [MEK, xf > 0.00, Flow < 0.1 kmol/hr, Value 0]
        [2Butanol, xf > 0.00, Flow < 0.1 kmol/hr, Value 0]
PPDS init: 2Butanol code 0 bp 372.66 Hvap 47.8762 Tc 536.01 Pc 4.23437e+06 Vc 0.
268558
PPDS init: MEK code 1 bp 352.73 Hvap 35.1384 Tc 536.78 Pc 4.26274e+06 Vc 0.26706
3
CHIPS Warning: PPDS returned some undefined constant properties
:              for component Hydrogen.
: all critical values are fine.
PPDS init: Hydrogen code 2 bp 20.38 Hvap 273.74 Tc 33.23 Pc 1.33344e+06 Vc 0.065
1613
 COMPOUND   38 HAS NO STORED UNIFAC STRUCTURE

   UNIFAC OR UNIQUAC CANNOT BE USED.
 NO ACTIVITY COEFFICIENTS ARE CALCULATED.
  ANY ANSWERS OBTAINED WILL BE IDEAL.

Design was successful!
Use 'print' or 'plot' to display the best process.

Complete Heat-Integrated Process Synthesis package (CHIPS) Version 0
$Revision: 9.2 $ $Date: 1995/04/26 12:28:32 $ by $Author: eric $
The feed is <1.0 A >.
Component descriptions:
Key  Component Name       Flow (kmol/hr)
  A: 2Butanol                    17.50
  B: MEK                         17.50
  C: Hydrogen                    17.50
Optimal solution  1 has cost $  68633.64.
Optimal sequence  1: u3[ u0[ 1.0 C + u0[ 1.0 B + 0.1 A ] ] ]
 1.  reactor1 UMI=[u3,c0,m0] Cost $ 6526.72
 2.    dist UMI=[u0,c0,m31] Cost $44128.06
         : product #2 <1.0 C >,  Cost $    -0.00
 3.      dist UMI=[u0,c0,m0] Cost $17978.86
           : product #1 <1.0 B >,  Cost $    -0.00
           : recycle #1 <0.1 A <0>>
```

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FIGURE 3

```
Component 2Butanol added with ID 0, label A, base flow 17.5 kmol/hr
Component MEK added with ID 1, label B, base flow 17.5 kmol/hr
Component Hydrogen added with ID 2, label C, base flow 17.5 kmol/hr
temp: not a valid keyword.
Feed (1 A ) defined.  Use 'show feed' to display.
CHIPS Warning: conv expects '( a ... )' with 8 entries but 1 found.
CHIPS Warning: comps expects '( a ... )' with 16 entries but 3 found.
CHIPS Warning: stoich expects '( a ... )' with 16 entries but 3 found.
Using unit 'reactor1': Well mixed isothermal reactor unit
                    nc (Number of special components) : 3
                  conv (Conversion rates) : 0.9 0 0 0 0 0 0 0
                  temp (Reactor temperature) : 723
                 comps (Components) : ( 2Butanol MEK Hydrogen                )
            conceptual (Level of design) : false
                excess (Excess of component required) : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0
               minflow (Minimum key flow) : 15
               recfrac (Recycle Fraction) : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
                stoich (Stoichiometry) : -1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0
             instrcost (Instrumentation cost) : 4000
               makeup (Amount of make-up allowed) : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0
               keycomp (Key component) : 2Butanol
                     k (Rate constant (expression in'x, the conversion)) : c c /(
1 -  c c )
              ldratio (Length/Diameter ratio) : 6
              maxflow (Maximum input reactant flow) : 100
                  rur (Recycle Unused Reactants?) : true
           limitequil (Reaction is limited by equilibrium) : true
                 cost (Cost function) : 1917 D^1.066
CHIPS Warning: toperec expects '( a ... )' with 4 entries but 1 found.
CHIPS Warning: botsrec expects '( a ... )' with 4 entries but 1 found.
Using unit 'dist': Ideal Distillation Unit based on FUG
                    rr (minimum reflux ratio) : 1.28
                    pm (pressure matching) : true
               toprec (tops recoveries) : 0.99 0 0 0
               botsrec (bottoms recoveries) : 0.99 0 0 0
                 stats (statistics) : 0 0 0 0
                    te (tray efficiency) : 0.38
                  name (a test for string vars) : Minerva
               reftemp (Enthalpy reference temperature) : -1
                   asr (Allow stripping/rectifying column designs) : true
              msindex (M&S Cost Index (280 for 1968)) : 288.4
              colcost (Column Cost function) : (1+(P>3.4)(0.0147(P-3.4)))(4.23 ms
index/280.0 7620 D (H/12.2)^0.68)
             traycost (Trays Cost function) : 0.61 S msindex/280 111.41 (D/1.22)^
1.9
            maintcost (Maintenance Cost function) : M ( colcost + instrcost + tra
ycost )
             instrcost (Instrumentation Cost function) : 4000
                 cost (Cost per year function) : TAX maintcost + (colcost + trayc
ost + instrcost)/     LIFE
               eduljee (Use Eduljee correlation instead of Gilliland) : false
          conceptual (conceptual) : false
No products yet defined.
 1.      [MEK, xf > 0.99, Flow > 15 kmol/hr, Value 0]
         [2Butanol, xf > 0.00, Flow < 0.5 kmol/hr, Value 0]
 2.      [MEK, xf > 0.00, Flow < 0.1 kmol/hr, Value 0]
         [2Butanol, xf > 0.00, Flow < 0.1 kmol/hr, Value 0]
PPDS init: 2Butanol code 0 bp 372.66 Hvap 47.8762 Tc 536.01 Pc 4.23437e+06 Vc 0.
268558
PPDS init: MEK code 1 bp 352.73 Hvap 35.1384 Tc 536.78 Pc 4.26274e+06 Vc 0.26706
3
CHIPS Warning: PPDS returned some undefined constant properties
:              for component Hydrogen.
: all critical values are fine.
PPDS init: Hydrogen code 2 bp 20.38 Hvap 273.74 Tc 33.23 Pc 1.33344e+06 Vc 0.065
1613
 COMPOUND   38 HAS NO STORED UNIFAC STRUCTURE

   UNIFAC OR UNIQUAC CANNOT BE USED.
 NO ACTIVITY COEFFICIENTS ARE CALCULATED.
  ANY ANSWERS OBTAINED WILL BE IDEAL.

Design was successful!
Use 'print' or 'plot' to display the best process.
+-------------------------------------------------------------------------------+
Feed stream 1.0 A @01 processed by 1st unit
Type 'reactor1' [3] description="Well mixed isothermal reactor unit"

Feed:
        Identifier:   1.0 A
        Flow:         17.5 kmol/hr
        Temperature:  372.0 K
        Pressure:     1 atm.
        State:        Liquid
  Recycle streams:
    1 : 0.1 A
  Product Specifications:

        Product 1: [code 0.1 A 1.0 B 1.0 C ]
        |                  Component |  m.f. | Flow (kmol/hr)
        |                  --------- |  ---- | --------------
        |                   2Butanol | 0.048 |         1.75
        |                        MEK | 0.476 |        17.50
        |                   Hydrogen | 0.476 |        17.50
        |                            |       |
        |        3 components, total | 1.000 |        36.75
        Temperature = 478.6, Pressure = 1.0, as liquid


  Unit design variables:

                          Diameter   : 1.98634 m
                       Temperature   : 478.619 K
             Adiabatic_Temperature   : 298 K
                            Volume   : 36.9444 m^3
                          Pressure   : 1 atm.
                       Reactor_Cost  : 3984.26 $
                  Heat of Reaction   : 0 kJ/hr
                            Length   : 11.9181 m
                   Conversion_Rate * : 0.9
                  Rate of reaction   : 4.26316 hr^(-1)

  Base unit cost: $     3984.26/yr


 Heat Transfer Requirements:
  HTR  1 : Heat  stream 0 from   372.0K to   478.6K at 1.0 atm. for 467558 kJ/hr
, flow 36.9444 kmol/hr
  HTR  2 : <empty>
```

```
+-------------------------------------------------------------------------+

+-------------------------------------------------------------------------+
Feed stream 0.1 A 1.0 B 1.0 C <0>@01 processed by 2nd unit
Type 'dist' [0] description="Ideal Distillation Unit based on FUG"

Feed:
        Identifier:   0.1 A 1.0 B 1.0 C <0>
        Flow:         36.75 kmol/hr
        Temperature:  478.6 K
        Pressure:     1 atm.
        State:        Liquid
  Product Specifications:

        Product 1: [code 1.0 C ]
        |                  Component |  m.f. | Flow (kmol/hr)
        |                  --------- |  ---- | --------------
        |                   Hydrogen | 1.000 |       17.50
        |                            |       |
        |        1 components, total | 1.000 |       17.50
        Temperature = 50.2, Pressure = 32.0, as liquid

        Product 2: [code 0.1 A 1.0 B ]
        |                  Component |  m.f. | Flow (kmol/hr)
        |                  --------- |  ---- | --------------
        |                        MEK | 0.909 |       17.50
        |                  2Butanol  | 0.091 |        1.75
        |                            |       |
        |        2 components, total | 1.000 |       19.25
        Temperature = 486.3, Pressure = 32.0, as liquid


  Unit design variables:

                        Reflux_Ratio   : 0.71575
                    Number_Of_Stages   : 11
                            Pressure * : 32 atm.
                                   Q   : 0.252668
                              Height   : 11.3575 m
                            Diameter   : 0.100386 m
                          ColumnCost   : 4509.07 $
                           TraysCost   : 7.06876 $
                  InstrumentationCost  : 4000 $
                      MaintenanceCost  : 170.323 $/yr
                     TotalCostPerYear  : 1021.94 $/yr
                        TopsRecovery   : 0.99
                     BottomsRecovery   : 0.99
                   Theoretical_Stages  : 4
               Reflux Ratio Multiplier * : 1.28

  Base unit cost: $      1021.94/yr


 Heat Transfer Requirements:
   HTR  1 : Cool  stream 1 from    320.6K to     50.2K at 32.0 atm. for 598630 kJ/h
r, flow 30.0256 kmol/hr
   HTR  2 : Heat  stream 2 from    486.3K to    516.1K at 32.0 atm. for 51471.9 kJ/
hr, flow 13.7782 kmol/hr
+-------------------------------------------------------------------------+

+-------------------------------------------------------------------------+
```

```
Feed stream 0.1 A 1.0 B <0>@31 processed by 3rd unit
Type 'dist' [0] description="Ideal Distillation Unit based on FUG"

Feed:
        Identifier:   0.1 A 1.0 B <0>
        Flow:         19.25 kmol/hr
        Temperature:  486.3 K
        Pressure:     1 atm.
        State:        Liquid
  Product Specifications:

        Product 1: [code 1.0 B ]
        |                  Component |  m.f. | Flow (kmol/hr)
        |                  --------- |  ---- | --------------
        |                        MEK | 1.000 |       17.50
        |                            |       |
        |        1 components, total | 1.000 |       17.50
        Temperature = 351.9, Pressure = 1.0, as liquid

        Product 2: [code 0.1 A ]
        |                  Component |  m.f. | Flow (kmol/hr)
        |                  --------- |  ---- | --------------
        |                  2Butanol  | 1.000 |        1.75
        |                            |       |
        |        1 components, total | 1.000 |        1.75
        Temperature = 369.9, Pressure = 1.0, as liquid


  Unit design variables:

                        Reflux_Ratio   : 1.41298
                    Number_Of_Stages   : 71
                            Pressure * : 1 atm.
                                   Q   : 0.216901
                              Height   : 47.8003 m
                            Diameter   : 0.746045 m
                          ColumnCost   : 62688.2 $
                           TraysCost   : 1962.11 $
                  InstrumentationCost  : 4000 $
                      MaintenanceCost  : 1373.01 $/yr
                     TotalCostPerYear  : 8238.04 $/yr
                        TopsRecovery   : 0.99
                     BottomsRecovery   : 0.99
                   Theoretical_Stages  : 27
               Reflux Ratio Multiplier * : 1.28

  Base unit cost: $      8238.04/yr


 Heat Transfer Requirements:
   HTR  1 : Cool  stream 1 from    351.9K to    351.9K at 1.0 atm. for 1.69762e+06
kJ/hr, flow 41.8471 kmol/hr
   HTR  2 : Heat  stream 2 from    369.9K to    370.8K at 1.0 atm. for 836679 kJ/hr
, flow 2.69526 kmol/hr
+-------------------------------------------------------------------------+
```

Chapter 6

Use of KBDS

6.1 Introduction

The need to provide a computerized design history is identified by Berzins and Jones as one of the key solutions to address the under-utilisation of people and resources during design, (Berzins and Jones 1989). This need will be discussed in this chapter. Three other key factors are also identified, an integrated process engineering system which is discussed in Chapter 7, the automation of engineering specifications and standards and the creation of a plant operating database. As the latter two factors are primarily the concern of the later phases of design they will not be discussed in detail here. It should be noted that CD-ROM issues of standards are now common place and, if available under an integrated environment, address the third factor. Finally factor four can be dealt with by modern plant control and data management systems that provide logging of key process parameters.

6.2 AI in process design.

The aim of AI is to develop computer systems that exhibit some of the intelligence characteristics of human beings. To this end techniques such as qualitative reasoning have been extensively studied to provide a framework for understanding how people reason about a problem. The tools and techniques developed in AI can be exploited to obtain design tools that also exhibit this type of behaviour and provide intelligent aids to the design process. Stephanopoulos gives a review of the use of AI in design and predicts a move towards a situation where human guidance is used to aid the computer to carry out significant portions of a design, (Stephanopoulos 1989). This prediction should be viewed against the current position where the computer is seen as an aid to the human. Tong and Sriram attempt to capture how AI can be utilised to aid design, (Tong and Sriram 1992), providing both a general overview and papers on specific applications in a wide range of fields. Key to the application of AI in design is the realisation that the manipulation of knowledge is critical to success. To this end various methodologies

have been proposed. The first applications to recognise the potential for a cross-over concentrated on knowledge-based, or expert, systems to capture expertise in specific areas. Dervakos et al consider such an approach to the development of a system to give the user guidelines for biocatalytic process design, (Dervakos et al 1989). For such systems there are three major programming styles, rule-based, object-oriented and access-oriented programming. Object-oriented programming tends to dominate due to the inherent modularity, flexibility and ease of maintenance. An object can either be a tangible physical entity or an intangible phenomenon. Objects are represented in frames and their attributes, or characteristics as slots in these frames. Slots can contain descriptive or procedural knowledge. Methods are used to send messages between objects and can be local or global. More recently it has been realised that to fully utilise knowledge handling advantages it is necessary to move away from expert systems with a very narrow focus towards developing a more general system modelling the design process. As discussed in Chapter 2, a large number of expert systems have been, and continue to be, developed but the application of more advanced AI techniques to design is now a more active research area. Much work has been done on capturing design, integrating tools, modelling the design process, controlling the design process and design automation. Tong and Sriram identify the AI issues associated with each of these with the overall aim being the automation of design, (Tong and Sriram 1992). AI issues identified are the use of object-oriented databases to capture design, representation and architectures for tool integration, taxonomy of tasks and corresponding methods to model the design process, how to control the design process, and machine learning and case based reasoning for design automation. Reference should be made to the extensive body of literature on AI techniques for discussions on aspects such as methodologies.

In order to move from the starting point of a design towards the desired end product it is necessary to take a series of decisions. At the start of a design there are a large number of possible outcomes within the solution space, each linked to a specific sequence of decisions. The solution space that is searched can become unmanageable if no attempt is made to impose a limit. Heuristics are commonly used to guide a design but the AI techniques of constraint management are becoming increasingly important.

Waters and Ponton describe work to address the problem of how to flag to the designer that proposed changes may effect earlier intent using an AI toolkit called Knowledge Craft, (Waters and Ponton 1992). Knowledge Craft is used as a DBMS for design knowledge that can maintain dependencies and warn of inconsistencies. This amounts to the application of truth maintenance in design which is a key element in an integrated design environment. Waters and Ponton view the design problem as being one of constraint satisfaction and concentrate on the representation of constraints. Checks are made to determine if the database contents violate any of the constraints but no further actions to remedy the violation are made. Knowledge Craft allowed the created tool to support the hierarchical nature of design with propagation of information between levels. Thus the knowledge associated with a block flow diagram can be traced through to the P&IDs. Whilst the DBMS is object oriented care was taken to ensure that the concept of an object did not focus on plant items alone.

6.3 Recording Design History.

One of the most pressing concerns with current design methods is the incomplete recording of an auditable trail that shows the evolution of the design. Frequently it is not clear why a decision was taken, what assumptions supported the choice made or how changes in basic data would affect the design product. Even after commissioning, no plant is a static entity and a lack of a full design history poses particular difficulties for those undertaking modifications as these may occur after those involved in the original design have moved on. Even if the original designers are still available it is highly unlikely that they will be able to remember sufficient detail to provide the necessary information. In addition to the initial design, all subsequent modifications must be equally well documented regardless of how trivial they appear to be. This is essential to maintain the audit trail and helps to allow the checking process to take place. Checking is necessary to verify that the design has been carried out correctly.

The problem of representing design history is discussed by Chung and Goodwin who present an Integrated Design Information System (IDIS) to address this issue, (Chung and Goodwin 1994). Three aspects of design history are supported by

IDIS: the exploration of design alternatives, the reasons for design decisions and design constraints. Given a set of design objectives and an initial design problem the actions of a designer can, in a somewhat simplified manner, be described as identifying alternatives, exploring them and selecting those which move towards the objectives. This description of the design process assumes that the objectives remain constant. Whilst this may be true for high level objectives, such as the type of material to be produced, in many other cases the objectives represent a moving target. During a traditional design the final design product is well documented, some issues raised are recorded, particularly in light of the formal review process currently undertaken, but the quantity of information on alternatives looked at and the reasoning behind the choices taken is variable. This missing information is termed the argumentation by Chung and Goodwin. If recorded it tends to be buried in a rather user unfriendly format such as the calculation files of the process engineer. These are the type of files that tend to be difficult to locate for old plants as they are the first victims of the rationalisation of records when space becomes limited. Even if available, the format is such as to make it difficult to locate the information required. As Chung and Goodwin point out the loss of information can lead to a loss of understanding of the design which, in the extreme, could result in modifications that jeopardise plant integrity and safety. IDIS is based on the assumption that the design process can be represented as the exploration of nodes in a network structure. Whilst moving away from the unrealistic linear representation, this approach implies discrete stages and points which could all be visited if sufficient time were available to explore the design space. The inherently cyclical nature of design is not addressed. Using a network representation can cause difficulties by forcing the designer into a certain pattern of working. This point is discussed further in section 6.4. IDIS uses the IBIS representation as a basis, as does KBDS. This representation is issue based. An issue can be any point where a decision is required, a problem arises or a question is raised. Raising an initial issue forms the basis of a network which expands to contain other issues as they arise. A number of alternative positions can be posted for each issue, if only one position arises then the issue ceases to be such and is resolved. Each position has arguments that can support or oppose it. Issues, positions and arguments form the basis of the IBIS network.

Positions and arguments can give rise to additional issues leading to a potentially complex tree like structure.

In addition to recording the argumentation via the IBIS representation, the assumptions and constraints applicable must be captured. Without this it is not possible to determine when choices and changes violate decisions taken earlier in the design. To address this point it is necessary to move into the field of truth maintenance.

IDIS has been implemented in Prolog to run on a SPARC station ELC and contains three basic components to capture the different aspects of design history. These are viewpoint, issue base and rule base. A viewpoint mechanism represents the design hierarchy in a chronological order but falls short of an Assumption-based Truth Maintenance System (ATMS). A strictly imposed chronological order could restrict a user as designers tend to "jump" around a design rather than execute it in a once through manner. The issue base is used to record the argumentation of the design and during the development of IDIS it was found to be necessary to add additional nodes and links to those present in the basic IBIS structure. Additional nodes include fact, comment and decision. Additional links include copy of, follow up, combined with and replaced. Many of the additions arose from the need to allow a number of designers to contribute to a design. An important issue to be addressed under such a system is the control mechanism that would be required for a multiple access system. Simply allowing everybody to add issues, positions, arguments etc could easily lead to confusion. Some form of mediation would be necessary. A rule based system is used to represent the design constraints. Rules are general, as defined by the system, or specific, as defined by the user, and aim to warn the user when a design constraint has been violated. Checking is not done automatically but at the request of the user to avoid unnecessary warnings of transient conditions. For this system to work effectively user discipline in initiating checking would have to be good. Failure to check runs the risk of the production of an invalid design.

Chung and Goodwin report on a test for the issue base within IDIS that involved the reconstruction of the history of a design rather than the recording of this information during the design process. As discussed in section 6.4 this is not a good test as a considerable degree of pre-knowledge can be applied to the structure

recorded. The test did, however, highlight additional links within IBIS necessary to represent real engineering problems. For example the "combined with" link resulted from the realisation that the representation could not support a partial solution needing to be added to another solution to create a viable overall solution. "Replaced" was added to allow the original issue to be superseded by a modified one. A concern here is that the network could rapidly become extremely messy for any reasonably sized problem. The new links resulted in concerns over temporal integrity leading to the addition of the "copy of" and "follow up" links. Careful consideration of the impact on overall history integrity is needed to avoid a situation where it becomes fragmented to the point of becoming useless. The proposed "replaced" link is unnecessary if a position can raise an issue and implies that only a single issue tree would be achievable under IDIS. This would represent a serious disadvantage and limitation of the system.

6.4 Project Management Systems

In order to make full use of available computer tools during a design it is necessary to manage both the data used and provided by the tools, and the application of the tools in an effective way. This is the goal of the integrated system tools discussed in Chapter 7 but it addresses only part of the functionality, that associated primarily with process engineering, required for the support of multi-discipline design tasks forces. To serve the multiple users inherent in such designs control of access and revisions is necessary. Additionally document control, progress monitoring and related project management functions must be supported. Available tools that address a number of these functions are discussed below.

6.4.1 CAE-System.

The CAE (Computer Aided Engineering) System was developed by Haldor Topsoe as an aid to the development and design of catalytic processes for the production of gases and the design of Ammonia and Methanol processes, (Christiansen 1991). There are three elements within the system; a data management system (IES), a drawing system and a programme library (GHEMB). Programmes within GHEMB (General HEat and Material Balance) were developed in-house as suitable commercial tools could not be found. They are implemented in such a way

that the user is presented with a common interface and can transfer data between applications. Data management via IES (Integrated Engineering System) was found to be necessary when the problem of linking GHEMB to a CAD package was investigated. To permit an automatic interchange of design data between the calculation packages and the drawing tool the stream and equipment identifiers used in the two places must be the same.

6.4.2 DICE.

The development of DICE (Distributed and Integrated environment for Computer-aided Engineering) was driven by the Civil Engineering discipline in response to failures in the design process that led to the deaths of 114 people when two walkways collapsed at the Hyatt Regency Hotel in Kansas City in 1981, (Tong and Sriram 1992). Errors in communicating intent and changes in the design were primarily to blame. To prevent such incidents occurring, what is required is a more adequate means of communicating between different disciplines within a firm and between firms. DICE aims to address this need with other objectives being:

(i) Capture of the history behind how a decision is reached including the information used, how it was used, and what was created.

(ii) Forecast the impact of design decisions on manufacturing and construction.

(iii) Interactively provide designers with planning information.

(iv) Develop intelligent interfaces for automation.

The focus of these is very much on large Civil Engineering projects but very much the same need exists within a process plant design team, although the automation of interfaces may be questionable in this case.

Advantages claimed for DICE are a reduction of errors in design, the sharing of design detail, improved planning, ease of recognition of design and manufacturing problems, designing for manufacturability and increased automation. To achieve this DICE uses object-oriented programming coupled with knowledge-based systems and DBMS. Negotiation is used to resolve a design decision that requires the input of two or more parties. The architecture of DICE includes a blackboard for communication, various knowledge bases and a means of control. At the time of

writing a prototype of DICE had been implemented and tested using the Hyatt Regency design as a test case.

6.4.3 ENGINES.

ENGINES was developed, in house, by John Brown Engineers and Constructors in response to a requirement identified during a business study. The aim of ENGINES is to create a database to store engineering data for a process plant in such a way that up-to-date information can be shared between disciplines. This was seen to have the benefits of improving the quality of deliverables and reducing the amount of internal rework undertaken. As with the ICI datasheet system, PROVUE, revision control is a key feature for ENGINES. The status assigned to data sets the access level, with the originating department only having access until a formal release is made. For Process Engineering ENGINES is used to specify streams, instruments, piping items, lines and equipment and to produce other deliverables such as the equipment list. ENGINES includes a link to an intelligent drawing package, AutoFLOW, also developed by John Brown. Information such as tag numbers and sizes can be exchanged. Eventually all departments within the company should have access to ENGINES with interfaces designed to fit their job functions. There are plans, (T.C.E. 1995), to link ENGINES with Du Pont's FES to create a Windows based expert system called FACET.

6.4.4 Plantool.

Plantool was developed to aid the concurrent design of large projects, (Hawtin and Chung 1996). Concurrent design is supposed to reduce the time and cost of design but without good control of information flow any advantage gained can be rapidly wiped out by the rework caused as definition is added to the design. Plantool attempts to address the problems inherent in concurrent design by planning a project in terms of the tasks that comprise it and linking support tools to these tasks. Project planning is implemented via a graphical interface that allows a hierarchical decomposition of the project into tasks and sub-tasks until a level is reached when the tasks can be defined in terms of the input information required and output information produced. Integration is provided by attaching applications to the I/O nodes of a task. Clicking on a node then activates the application.

Plantool has document control aspects to support multi-user access, version

control, dependency checking and node history. Dependency checking simply flags a list of tasks that are effected, and require re-examination, when the output from another task changes. The node history records information such as the initiator and tool used each time a node is activated. Design history is recorded via IBIS, discussed in Section 6.3.

6.4.5 POINTER.

POINTER (People Oriented InformatioN Tracking for EngineeRing) was developed at Loughbrough University in collaboration with British Gas, (Das et al 1995). The inability of organisations to handle data effectively had been identified as a major obstacle to the completion of projects and to competitiveness. POINTER is based on the assumption that not all data has to be centrally controlled, as long as there is effective local control. This is termed a federal, distributed, data management system. All data is classified as structured, that which can be easily identified and described, and unstructured. The two types are then handled by separate elements of the system, that for unstructured being a data management engine specifically developed for POINTER. At the time of writing Das and co workers had implemented the data handling aspects of POINTER at a local level but had not tackled the sharing of this data between multiple users.

6.4.6 WinCoordinate.

The exchange of information between disciplines is identified as key to the success of a project, (Jalali-Ghazaani 1996), and traditional means of handling, by paper, as resulting in the need for multiple re-entry of data. This leads to the possibility of transcription errors and to the existence of a number of revisions of data in circulation with the attendant possibility of some parties working with out of date information. WinCoordinate is a blackboard system for the exchange of information between disciplines aimed at overcoming these difficulties. It features password protected access to prevent un-authorised access to a project area with a hierarchy of access, the project manager having the highest level of priority. The features described by Jalali-Ghazaani and co workers are very much like those present in ENGINES.

6.4.7 Zyqad.

Whilst officially termed Process Workbench, with the company name being

Zyqad this tool is commonly referred to by this name. Zyqad is the result of work undertaken to address an identified industrial need to develop computer methods to support the complex and creative nature of front end, conceptual, design. The basis of the system, the OPUS suite of tools, is described by (McBrien et al 1994). Zyqad has now been developed to the stage where it is being used by industrial consortium partners, such as Foster Wheeler, for actual design work. One reported use is linked with the STEP initiative discussed in Section 2.3.6.

The conceptual phase of a project was focused on during the development of OPUS as this had been identified as key to obtaining satisfactory safety and environmental impact, operational behaviour and economic performance with minimal design cost impact. McBrien and co workers saw that the use of computers to perform individual design calculations had reached the limit of ability to provide further improvements to the design process and pointed to integrated systems as the way forward. They saw expert, or knowledge-based, systems as providing the key to this, thus OPUS and Zyqad have this basis. OPUS has a fairly standard expert system architecture of knowledge base, database, inference engine and graphics driver. An object oriented approach is used.

As the focus is on conceptual design, the database key used by OPUS is the PFD representation but this is extended in Zyqad to cover P&IDs and service the later stages of design. QA concerns are addressed by having all items chained back to the drawing to provide an auditable trail. Data exchange standards are conformed to making it possible for the user to utilise any preferred tool and still only enter data items once. If a data item used by an application has changed the most up to date value available is automatically used when the tool is next activated.

One element that is not well covered by existing tools is the recording of design history. This is essential to provide an auditable trail for a project and to enhance the learning experience.

6.5 KBDS

KBDS is intended as a computer-based support tool to assist a group of designers undertaking a process design. It is implemented in CLOS with the GUI

using LispView. The representation of the design process used in developing KBDS is based on the exploration based model of design proposed by Smithers, (Smithers et al 1990). Bañares-Alcántara discusses the alterations made to the basic model and highlights the ability to support the exploration of design alternatives as a key improvement, (Bañares-Alcántara 1991a and 1991b). The AI technique of Assumption based Truth Maintenance Systems (ATMSs) are used to support this exploration by recording the dependencies of equipment and schemes. The design is represented within KBDS as three interrelated networks that evolve as the design progresses. One network is for design alternatives, one for the models of these alternatives and a third for design constraints and specifications, (Ballinger et al 1994). King and co workers describe the third element that allows the recording of design intent, (King et al 1995). This is linked to the alternatives history and allows any user to determine how the design decisions taken were arrived at. If any factors instrumental in a decision change, backtracking allows the affected decisions to be revisited and checked. A more promising position from that originally chosen could arise under the changed conditions. This work is also discussed by (Bañares-Alcántara et al 1994). In addition to the basic IBIS network elements two new objects were found to be necessary during implementation in KBDS, steps and tests. Steps are transformations of a design alternative suggested by a selected position and allow back tracking should a designer wish to do so. Tests allow constraints to be placed on design alternatives and can be used to flag violations that occur during the design. As such tests move towards truth maintenance capabilities which would be a key feature during conceptual design. Within KBDS the IBIS network is generated and manipulated by the Intent Tool. Bañares-Alcántara and co workers highlight three ways in which this tool can be used to aid the designer:

(i) The design intent, or rationale, is stored in such a way that backtracking is possible when a design factor is changed.

(ii) Positions can be automatically evaluated by weightings given to the associated arguments.

(iii) Reports describing the evaluation of a design can be automatically generated.

The goal in developing KBDS was to provide an intelligent assistant to the process designer, (Ballinger et al 1994). Important tasks for an intelligent assistant were identified as being to remind a designer what they are trying to do and what has already been done. The assistant should not attempt to take over complicated activities that are not well defined and fall outside the range of expertise. KBDS aims to allow the designer to concentrate on creative aspects by taking over routine tasks.

Of the three trees within KBDS the alternatives tree can be said to be the central element for recording the progress of the design. The tree develops along the lines of a hierarchical model of design starting with a single "black box" and progressing to a completed design. Refinement, addition of detail, and decomposition, splitting into sub systems that can be worked on by separate designers, can occur. The models tree is directly linked to the alternatives tree but more than one model can be associated with an alternative. This arises from exploration of the alternative by tools such as standard process simulators. The intent tree also evolves during a design but it could be argued that the tree structure identified by (Ballinger et al 1994) is not directly applicable in this case. Whilst each issue raised undoubtedly results in a tree like structure, a design will not start with a single issue that is posted by the user and subsequently refined to give a single intent tree for the whole design. In fact such a tree would rapidly become unwieldy and almost impossible to successfully negotiate. The major advantage of recording intent, of having an accessible, auditable trail, would thus be lost. A more realistic model of intent is that numerous, apparently random issues would be posted by a designer during the early stages of design each with a resultant tree. The interrelationship of the trees may only become apparent at a later stage. Any aid to a designer must be able to support this pattern of unstructured thinking, akin to using Post-it stickers to remind a designer of things to remember, that occurs during the creative stages of design. During case study work, discussed below, the KBDS intent tool was not found sufficiently flexible to do this.

Each argument can only support the position with which it is associated. Weightings can be assigned to arguments in order to obtain a rough ranking of positions and so aid the decision process.

Reports can be automatically generated to cover the evolution of one design alternative to another and the process, termed the argumentation, that resulted in a given decision.

6.5.1 Limitations of the tested version KBDS.

KBDS is not a standalone tool containing all the features necessary to support design but forms part of a suite of tools. A primary interface is with épée, discussed in Chapter 7, which acts as a means of integrating applications. During the duration of this work the interface was not fully functional, severely limiting the functionality of KBDS. When used independently of other tools the utility of KBDS is limited to the somewhat artificial creation of a design history, this process should be intimately linked with undertaking the design.

In KBDS a small triangle next to a button in a view indicates the presence of a pull down menu that can be brought up by a single press of the right mouse button. Other features used in views are that if any option is unavailable it is dimmed and that a line of dotes next to a menu item indicates that another window is displayed if it is selected. All windows have either a pull down menu icon or a pin shown in the top left hand corner. Left clicking on the pin removes the window. The pull down menu allows standard window operations such as resizing, moving, refreshing and quitting to take place.

6.5.2 Case study work.

The initial phase of the HF case study was used as a test case for using KBDS. No user manual was available for the tool but it was found to be relatively easy to navigate around without this but some of the nuances of functionality may well have been missed. This is best reported by looking at the use of the various windows available.

6.5.2.1 Top Window. The first activity undertaken when setting up a new project within KBDS is to complete the project, metascheme and scheme information shown in the Top Window, Figure 1. Assigning a unique project name ensures segregation of project histories. Each project can consist of one or more metascheme, covering major processing alternatives, and each metascheme can have one or more scheme, covering alternatives within a processing route. For the HF case study this distinction between metascheme and scheme was not found to be particularly

necessary or helpful as the three options being considered vary only in means of acid feedstock provision. The three options were each set up as a metascheme, PROCESS0, PROCESS1 and PROCESS2, each with a single scheme but the set up chosen could equally well have been that of a single metascheme with three schemes. The use of three metaschemes was chosen in this case so that three separate history strands were produced. The three tier structure would be necessary for projects where more than one processing route is available to the product, each with variations such as the means of feeding one of the main components.

There are five pull down menus available within the body of this window.

i) KBDS. Contains the options to Start, End or Refresh the run. Starting via this route was not available at the time of testing.

ii) Project. Contains the options Browser, Load, New, Dump and Unload-Project. Dump was found to be most important as this was the means by which the work input into a project could be saved to file. Load allows a project stored outside the system to be loaded onto it. New is the first step in creating a new project. Unload can be used to save a project outside the system. The Browser option was not available at the time of testing.

iii) Metascheme. Contains the options Browser, Create and Current. Browser brings up the Metascheme Browser, Figure 2, which is discussed below. Create allows a new metascheme to be added to the project. Current brings up the Current Metascheme window. This shows a list of all the metaschemes defined for the project and allows the deletion of any that are unwanted. A Show button can be used to view the MetaSchema Browser before any changes are made. If a mistake is made there is an option to restore the situation prior to applying the changes and returning to the Top Window.

iv) Scheme. Contains the options Browser, Create, copy, Save, View, Flowsheet and Print. Browser brings up the Schema Browser, Figure 3, which is discussed below. Create allows a new scheme to be added to the metascheme. Copy is as discussed under the Design History window below. Save allows an unsaved scheme to be saved, otherwise this option is dimmed. View brings up a view of the selected scheme, Figures 6, 7 and 8. Flowsheet brings up the Flowsheet Tool, discussed below. Print brings up a menu that allows the scheme to be printed to file

or as a hard copy in either portrait or landscape format.

v) History. Contains the options Design and Objectives. Design brings up the Design History window, Figure 4, which is discussed below. The objectives option was not available at the time of testing but this would be a prime location for a link to the Intent Tool.

Given the importance of the Top Window it was found to be irritating that the Intent Tool automatically opened directly over it when KBDS was started and had to be closed or moved before access could be gained to the Top Window. A more preferable way of accessing the Intent Tool would be to call it up via a button as and when required. As tested the Intent Tool was not fully integrated into the KBDS GUIs.

6.5.2.2 Browsers. The MetaSchema Browser, Figure 2, shows all the metaschemes for a given project along with the schemes associated with the highlighted metascheme. Figure 3 shows the equivalent window for schemes, the Schema Browser, this can be accessed from the Scheme pull down menu on the Top Window or by using the "Show" button when a scheme is selected in the Metaschema Browser. Here all the schemes associated with a project are displayed and for the selected scheme the parent metascheme and constituent units are shown. In this window schemes can be saved, created, copied and viewed. The Metaschema Browser for the parent metascheme can also be viewed using the "Show" button but the Units Browser had not been implemented in the version of KBDS used.

Using these browsers it was simple to navigate around a project, a feature that would become increasingly important as more information was entered into the system, using the "Show" buttons to move to the required document. Some features had not been incorporated into the version of KBDS used but this was not found to be a significant problem.

6.5.2.3 Design History. The history of a project can also be directly accessed from the Top Window. Figure 4 shows the Design History window with the schemes available for the metaschemes shown as separate starting points for the evolution of a history. A more complex example, taken from Cassidy, is shown in Figure 5. Clicking on a scheme with the left button brings up the view window for that scheme, Figures 6, 7 and 8 are print outs of this window for the three options under

consideration. Using the right button displays a menu which also allows access to the view window but additionally has the following items:

i) Flowsheet. Brings up the Flowsheet Tool.

ii) Hide Successors. Used to simplify a complex tree by hiding part of it. If this has been done previously the menu changes to include "Show Successors".

iii) Copy. Brings up the Copy Scheme window that takes a copy of a saved scheme so that it can be modified and evolve into the next generation. This is also accessed under the Copy button on the Schema Browser and from the Scheme pull down menu on the Top Window.

iv) Save. Saves a scheme that has not been saved elsewhere, otherwise dimmed. Once saved a scheme forms part of the design history and cannot be changed.

v) Description. Brings up the Description Editor, Figure 9, which permits a description of the block to be entered. This should be stamped with the name of the person who created it but this did not occur in this case and a default name, Geoff, was added. For multiple user systems name stamping is an important part of ensuring that an auditable trail exists.

vi) Reports. Brings up the Report Generator window, Figure 10. This allows the options to be set for the contents of the automatically generated report. Also accessed under the Issues pull down menu in the Intent Tool.

vii) Delete. Allows only unsaved schemes to be deleted, otherwise dimmed.

viii) Print. Pulls up the print menu.

During testing problems were encountered with this pull down menu as it had a habit of freezing up. When this occurred the menu remained on the screen and could not be deleted without restarting KBDS.

6.5.2.4 Flowsheet Tool. The Flowsheet Tool in KBDS has a functionality that exceeds that of simply being a means by which to draw the views associated with each scheme. Although gaining such a representation, from the simple block flow diagrams shown in Figures 6, 7 and 8 to PFD, is important, if this were the only purpose it would be better served by a link to a commercial drawing package which

would give much better functionality. There are three pull down menus available in this window:

i) Edit. Contains the options Select Units, Select All, Delete All Units, Refresh, Grid and Grid Size. These are all related to drawing functions.

ii) Flowsheet. Contains the options Reset, Load and Mode. Load allows schemes other than the current one to be brought into the Flowsheet Tool to be worked on. Mode brings down a menu that allows an unsaved scheme to be swapped into edit mode, modifies the information displayed and configures an unsaved scheme. The functionality of Reset was unclear during testing.

iii) Scheme. Contains the options Alternatives, Apply Methods, Save, Copy, Decompose and Print. Alternatives brings up a menu containing all the alternative schemes available under the metascheme and allows the user to move to any of these. Apply Methods brings down a menu of the tools available for application to the scheme and will be a very useful feature of KBDS when fully implemented. At the time of testing only ASPEN was available. Save permits an unsaved scheme to be saved, otherwise it is dimmed. Copy brings down the Copy Screen window discussed previously. Decompose allows an unsaved scheme to be split and forms part of the means of creating a branched history. A scheme to be decomposed must first be copied to create a descendent and this descendent is then split, each part having the same parent in the design history. An example of the use of this functionality would be splitting a simple black box diagram into a strand for the reaction area and one for the separations area. Print brings up the standard print menu.

6.5.2.5 Intent Tool. This tool is the key novel feature of KBDS as it allows the reasoning behind the direction that a design takes to be recorded. Perhaps because it was an unfamiliar way of working it was found to be extremely difficult to determine the best way of starting off recording the issues, positions and arguments that constitute this reasoning. Because of these difficulties a number of false starts were made and a large tree was not produced. Figure 11 shows the most promising starting point uncovered, that of treating each separate scheme as a starting point for a hierarchy of issues. A draw back of this representation would be that issues down the path that was not selected would always show up on the block menus and could

always remain unresolved unless the user forced their resolution. It could equally well be argued that there should be a single starting issue for each design as there must have been at some point a single question that led to the design of each plant in existence. One possible problem with this approach is that in most cases recording of design history will not start until sometime after this question has been posed leading to the need to invent a considerable amount of history. Another could be that a single tree for a complete design would rapidly become very large and unwieldy. There is the ability to find a given part of a tree built into KBDS but this does not solve the presentation problems. With the test case, once a starting point had been decided it was found to be difficult to layout the intent tree in a way that was easy for the user. Additional elements had to be manually placed and as the form of the tree could not be prejudged this rapidly led to the potential for overlap and a break down in the hierarchical structure of the tree. Building such a tree on a grid similar to that used in a spreadsheeting package is easier as the lining up of elements at the same level is simplified, as is the inclusion of additional space in the working area. Figure 12 shows an evolution of Figure 11 to include positions and arguments related to the Feedstock issue under Block 1.

A single click with the right mouse button on the background of the Intent Tool window brings up a menu containing the options listed below:

i) Add Node. This allows the various elements, issues, positions, arguments etc., needed to build the tree to be input. The created node then has to be manually placed and a link made to whatever it relates to. A more convenient way of doing this would be to allow the user to highlight the node to which the new node was to be related, specify the manner of the connection and have the system automatically place the new node.

ii) Find. Brings down a list containing various options to help the user to uncover information about the status of the issues within the tree. In addition to a list of all issues, separate listing of resolved and unresolved issues can be provided. For a given issue a ranked list of positions can be provided or just the best position displayed. If there are any problems with any issues these can also be listed. This feature would be useful when truth maintenance features are included.

iii) Locate Issue. This aids navigation around the tree by bringing up a list

of issues and moving to the one that is highlighted.

iv) Move Selection. This option was not functional during testing and attempting to use it caused problems that led to the need to restart KBDS.

v) Show Map. Brings up the Intent Map which can be used to see the overall structure of a complex tree without being able to see the detail. The utility of this feature is questionable.

Each node in the tree each has a menu associated with it which is brought down by a single click of the right mouse button. The initial menu is the same for all nodes, containing Find, Select, Description, Disconnect Node and Delete Node, but the sub-menus vary between node types. This is primarily related to the Find sub-menu which contains node type specific information. For example for a block predecessors, successors, positions and issues can be found, but for issues it is ranked positions, best position, potential problems, position evaluation and a report that can be displayed. Position evaluation allows weightings to be assigned to the positions available for an issue and is key in ranking positions in order to determine which would be the best to adopt. Description brings up a Description Editor window for the node and allows a brief paragraph of text to be entered. Figure 13 shows an example for an issue.

6.5.2.6 Functionality. The version of KBDS tested was an early research version that cannot be expected to have the degree of user friendliness that would be required from a commercially available tool but should contain the functionality. KBDS was not found to be extremely robust during case study work, with an irritating tendency to crash and cause the loss of many hours of work. Part of the problem was that the routine for saving was not intuitive or easy to use. Such problems would rapidly put potential users off and the programme needs to be made much more user friendly, not just for general use but also to allow a fair and complete evaluation of functionality to take place. Additionally the loading procedure took a considerable amount of time, between two and five minutes, and caused a high number of warning messages to be displayed. This would be guaranteed to worry the user.

The structure of the windows within KBDS is complex but was found to be such that it was easy to negotiate around. Rather than having a single way to reach many views the comprehensive pull down menu structure gives the user a number of

options to chose from if, for example, wanting to access the view window for a scheme. This gives the flexibility of allowing each user to determine their preferred way of using the system but may confuse the novice user.

It was found to be very difficult to generate an adequate intent tree and a number of false starts were made. A lesson learnt from these was that it was extremely important to take care when wording issues to ensure that the tree evolved in a way that was easy to follow. Part of the problem may have been an unfamiliarity with working in this manner but it did highlight a limitation of KBDS in that it was not possible to create an ancestor issue, only a descendent. This attempts to force the design into a linear structure whilst in practice, particularly during the early stages of design, the generation of issues is a significantly more random process. A greater degree flexibility in generating the issue structure of the intent tree is necessary. The environment in which the tree is created should be modified so that it is easier to both line up elements and add in additional space as necessary.

Truth maintenance features had not been implemented in the version of KBDS tested but this functionality is seen as a key potential selling point for the tool. The ability to check if assumptions have been violated when firm information becomes available would be very useful during design. Inherent in this should be checks that the plant remains within the permitted legal framework, e.g. emission limits.

Whilst the deletion of unconnected nodes mentioned by Cassidy as a future development is a sensible measure to allow users to recover from errors, careful thought needs to be given to the requirement for additional deletion capabilities. To be fully effective in a design team each member should be able have access to KBDS raising concerns over control of the structure. Within the intent tree, whilst the ability for every engineer involved in a design to delete issues and their associated documentation would be a cause of potential chaos, having a manager with the ability to do this may be essential to keep the tree in a serviceable form. This raises the issue of access control and setting different privileges for different users. A possible structure could be based on the system used for Lotus Notes Team Issue databases. On this model there would be four levels of access:

i) Editor. Acting as a moderator and with the ability to edit and delete all

documents, flowschemes, issues, positions and arguments etc, as well as create them.

ii) Author. With the ability to create all the documents but only able to edit those which they created. No deletion rights.

iii) Commentator. Able to create positions and arguments only, but able to edit those which they created. No deletion rights.

iv) Read Only. Only able to read documents.

To protect the validity and confidentiality of data held within KBDS access would have to be controlled. Within the case study it was not possible to address multiple user issues.

6.6 Conclusions

A tool that fully captures design history is essential to serve a design methodology, such as that described in Chapter 4, that is based on treating design as a creative exploration of alternatives. To progress a design within a reasonable time frame it is not possible to fully explore all the alternatives that are generated but it is important to record them. This allows back tracking should it be found that the design has ended up in a blind alley or if sufficient time is available at a later date, possibly for another plant, to allow optimisation to take place. Inherent in recording the history of a design is the evolution of flowsheets and the reasoning behind the decisions taken. KBDS is one of the few tools that addresses these issues. The provision of truth maintenance to allow checking for the violation of assumptions is an added bonus. However, to fully exploit the potential integration with other design tools it is essential that the recording of design history becomes an inherent part of the design process.

Several specific points that need to be addressed were uncovered during case study work. It must be possible, as pointed out by Cassidy, to have arguments that disagree with as well as support positions. This avoids the need to "play" with the wording of elements within the intent tree so that the weights assigned support the strongest position in the manner intended. To maximise utility, issues related to control and access to data within multiple user systems need to be addressed.

FIGURE 1

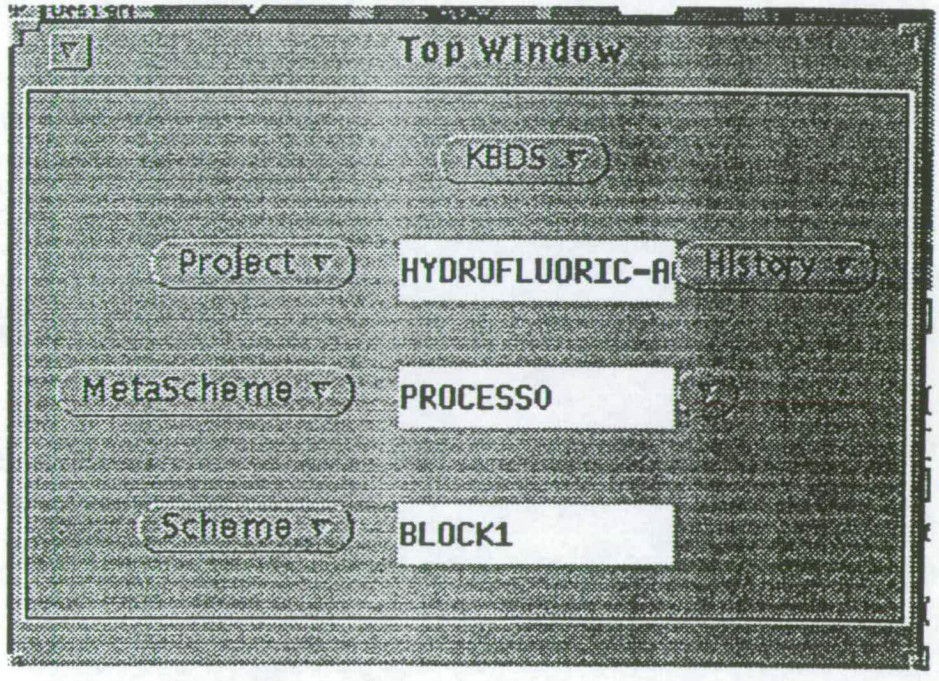

Top Window
KBDS
Project
HYDROFLUORIC-A
History
MetaScheme
PROCESSO
Scheme
BLOCK1

FIGURE 2

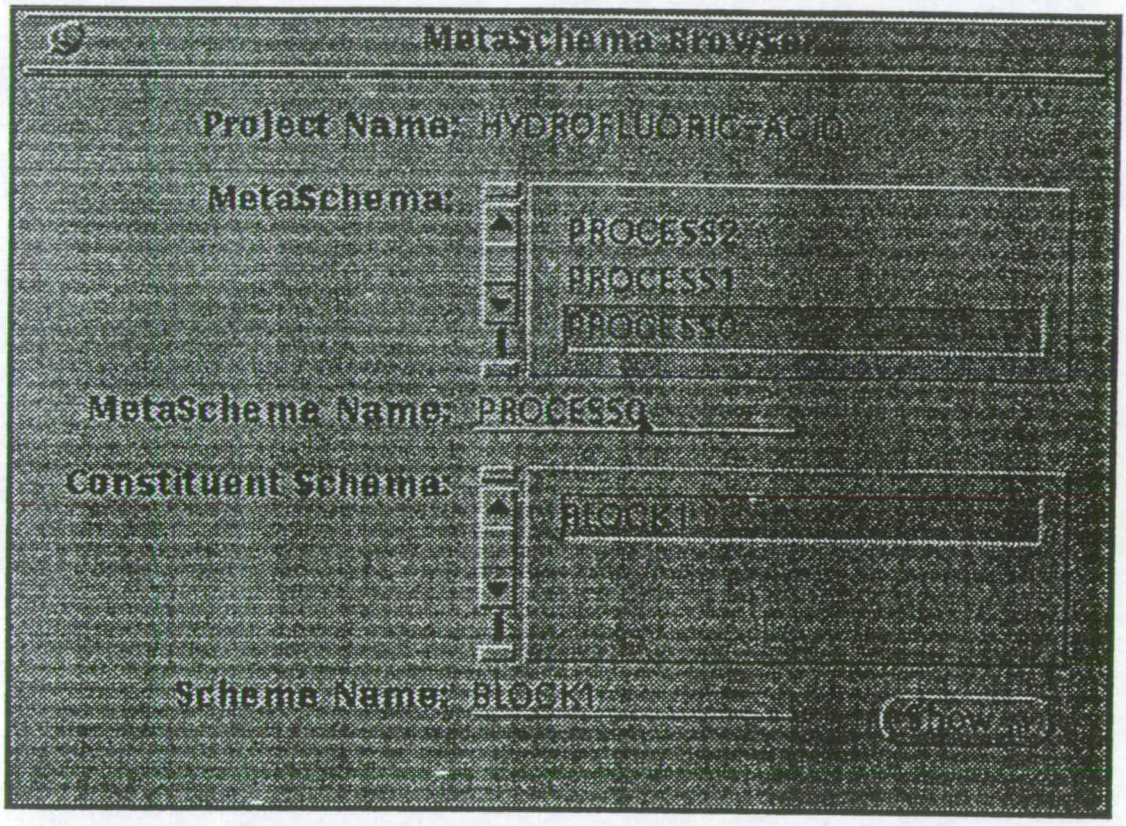

MetaSchema Browser
Project Name: HYDROFLUORIC-ACID
MetaSchema:
PROCESS2
PROCESS1
PROCESS0
MetaScheme Name: PROCESS0
Constituent Schema:
BLOCK1
Scheme Name: BLOCK1

FIGURE 3

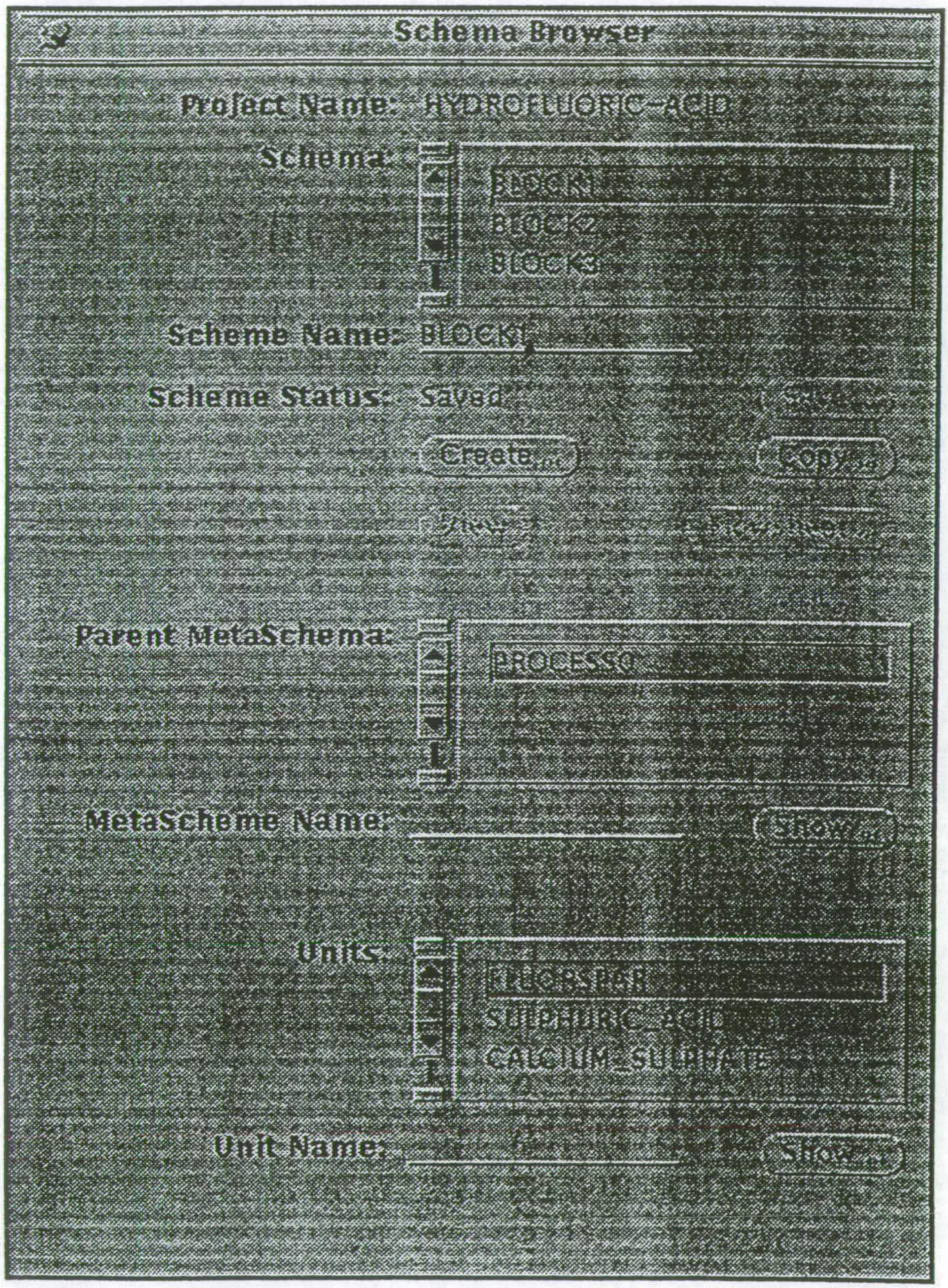

Schema Browser
Project Name: HYDROFLUORIC-ACID
Schema:
BLOCK1
BLOCK2
BLOCK3
Scheme Name: BLOCK1
Scheme Status: Saved
Create...
Copy...
Parent MetaSchema:
PROCESSO
MetaScheme Name:
Show...
Units:
FLUORSPAR
SULPHURIC_ACID
CALCIUM_SULPHATE
Unit Name:
Show...

FIGURE 4

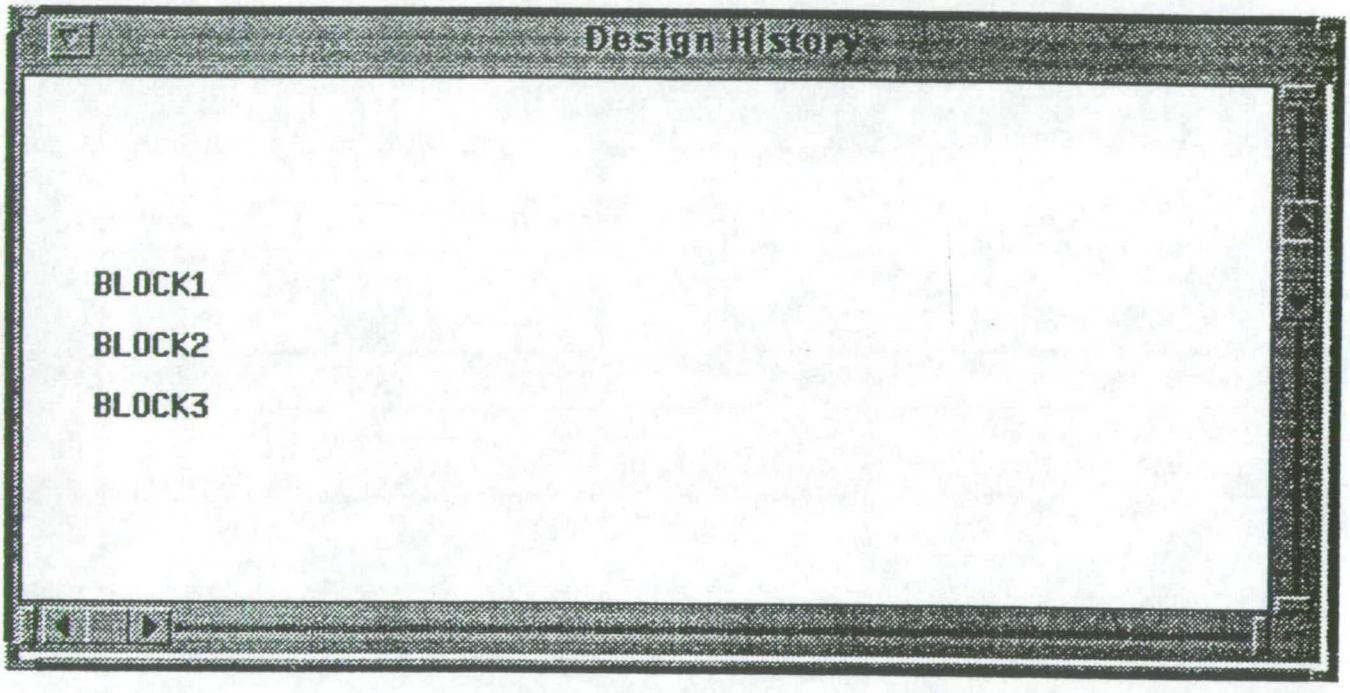
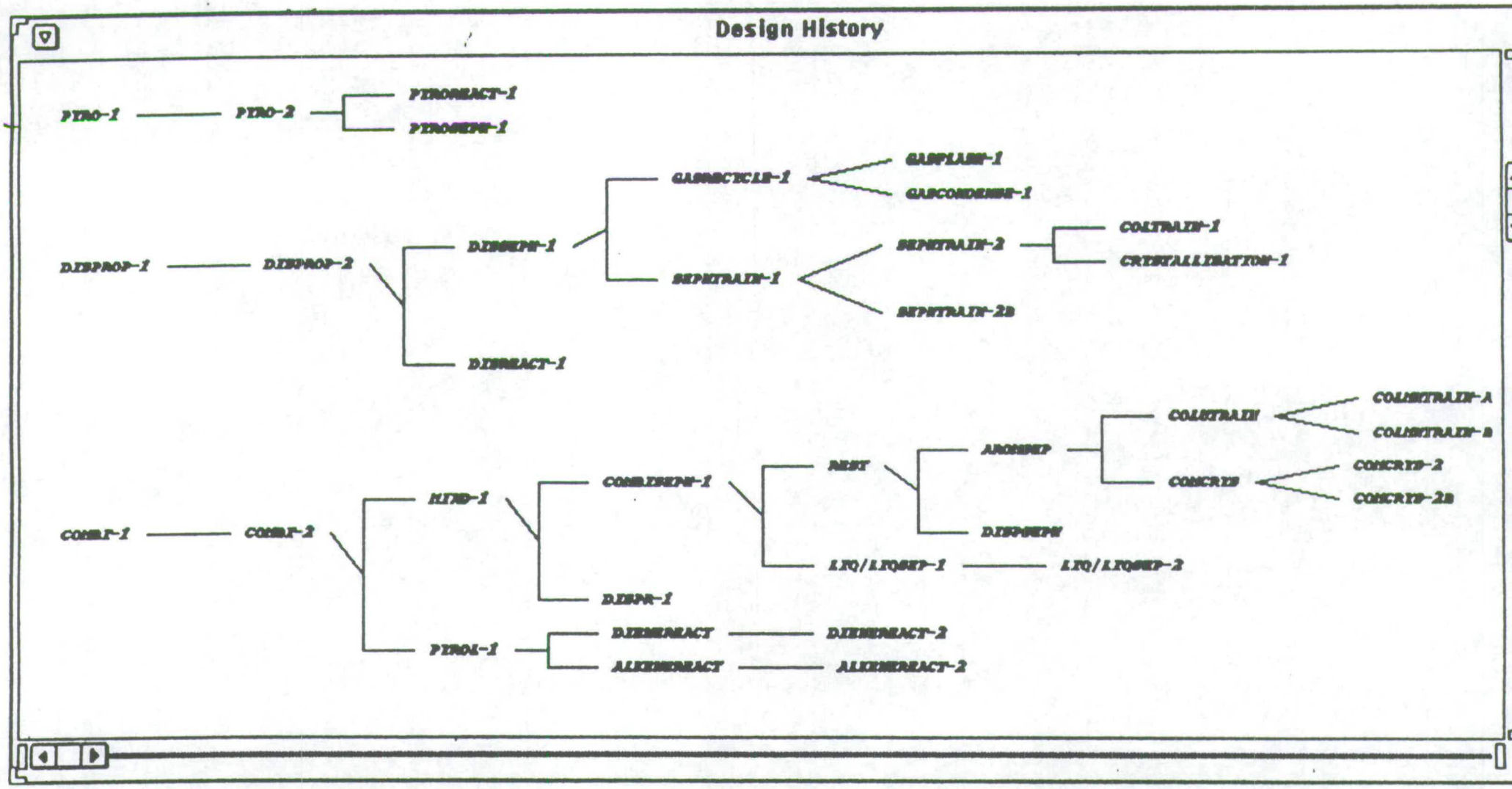
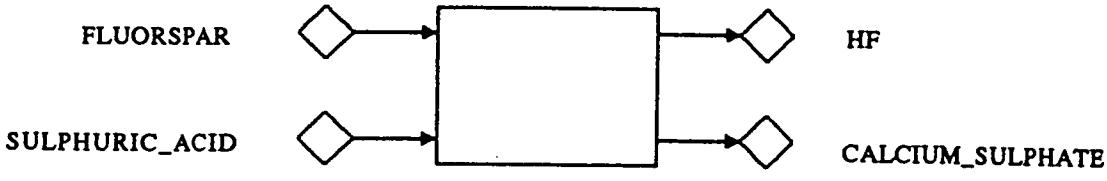


FIGURE 5

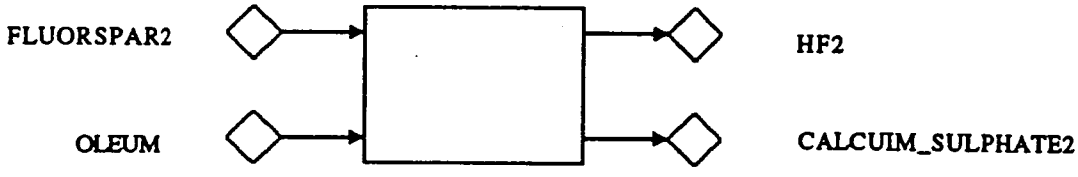

Design History
PIRO-1
PIRO-2
PIROREACT-1
PIROSEP#-1
DISPROP-1
DISPROP-2
DISSEP#-1
GASREACTOR-1
GASPLANT-1
GASCONDENSER-1
SEPNTRAIN-1
SEPNTRAIN-2
COLTRAIN-1
CRYSTALLIZATION#-1
SEPNTRAIN-2B
DISREACT-1
COMB.F-1
COMB.F-2
MIXD-1
COMBUSER#-1
REST
AROMSEP
COLSETRAIN
COLSETRAIN-A
COLSETRAIN-B
CONCRYS
CONCRYS-2
CONCRYS-2B
DISP#SEP#
LIQ/LIQSEP-1
LIQ/LIQSEP-2
DISPAR-1
PIROL-1
DISSEPARACT
DISSEPARACT-2
ALKSEPARACT
ALKSEPARACT-2

BLOCK1



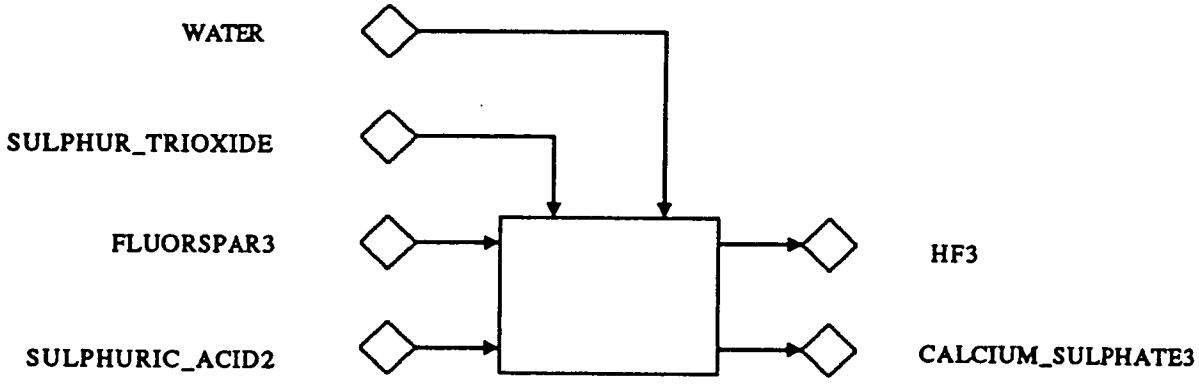
BLACK_BOX

BLOCK2



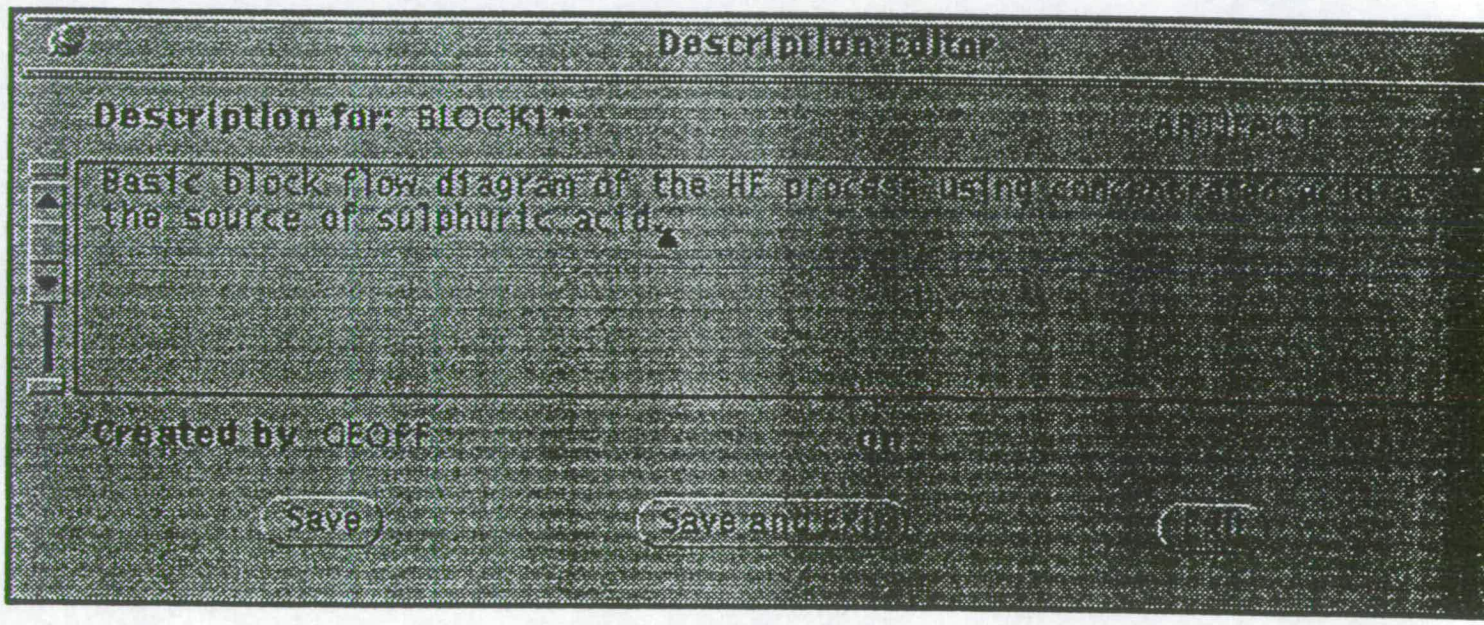
BLACK_BOX2

BLOCK3



BLACK_BOX3

FIGURE 9


Description editor
Description for: BLOCK1*
Basic block flow diagram of the HF process using
the source of sulphuric acid
Created by GEOFF
Save
Save and Exit

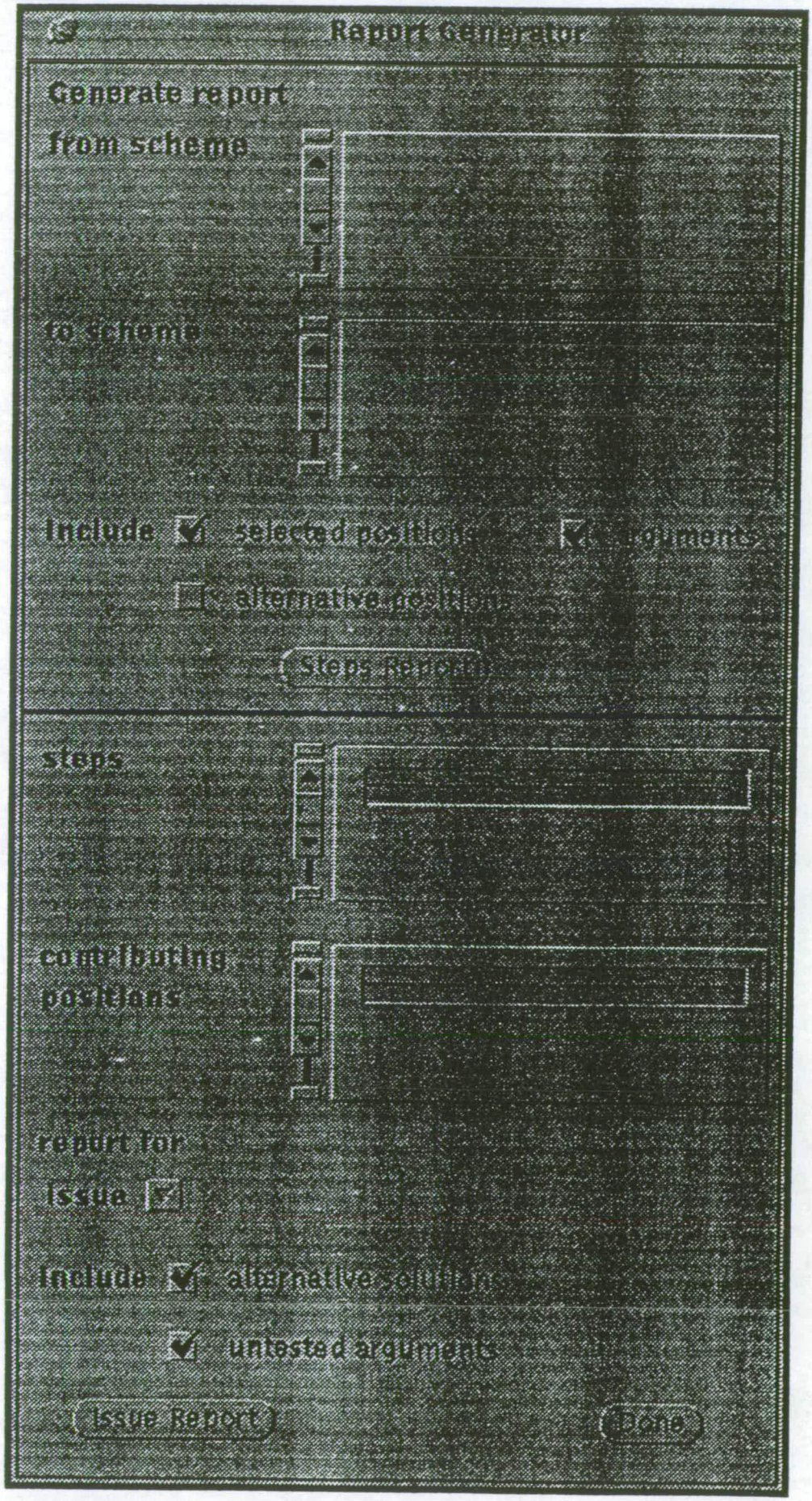

Report Generator
Generate report
from scheme
to scheme
Include selected position
arguments
alternative position
Steps Reported
steps
contributing positions
report for issue
Include alternative solution
untested arguments
Issue Report
Done

FIGURE 11

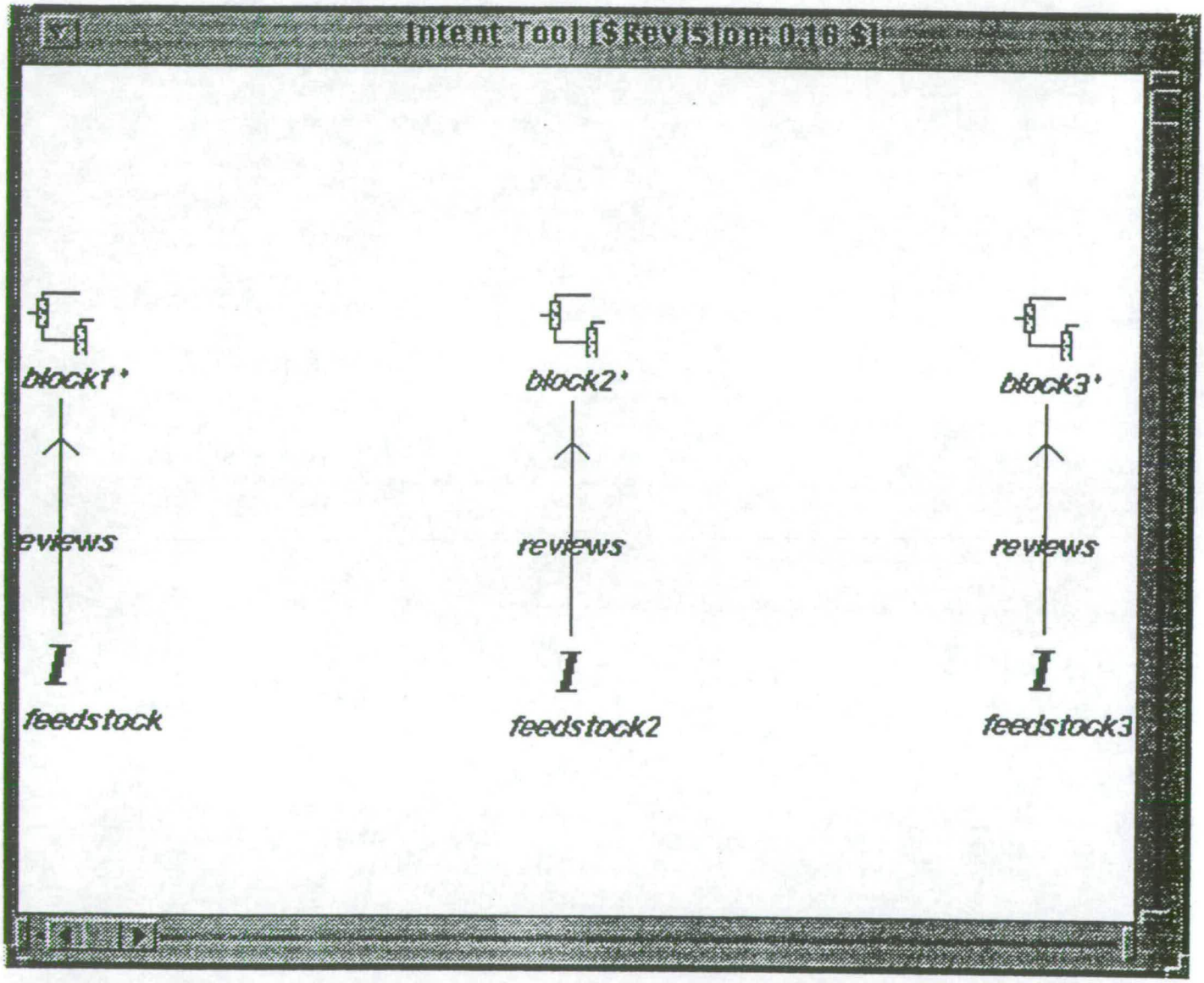

Intent Tool [$Revision: 0.16 $]
block1*
eviews
feedstock
block2*
reviews
feedstock2
block3*
reviews
feedstock3

FIGURE 12

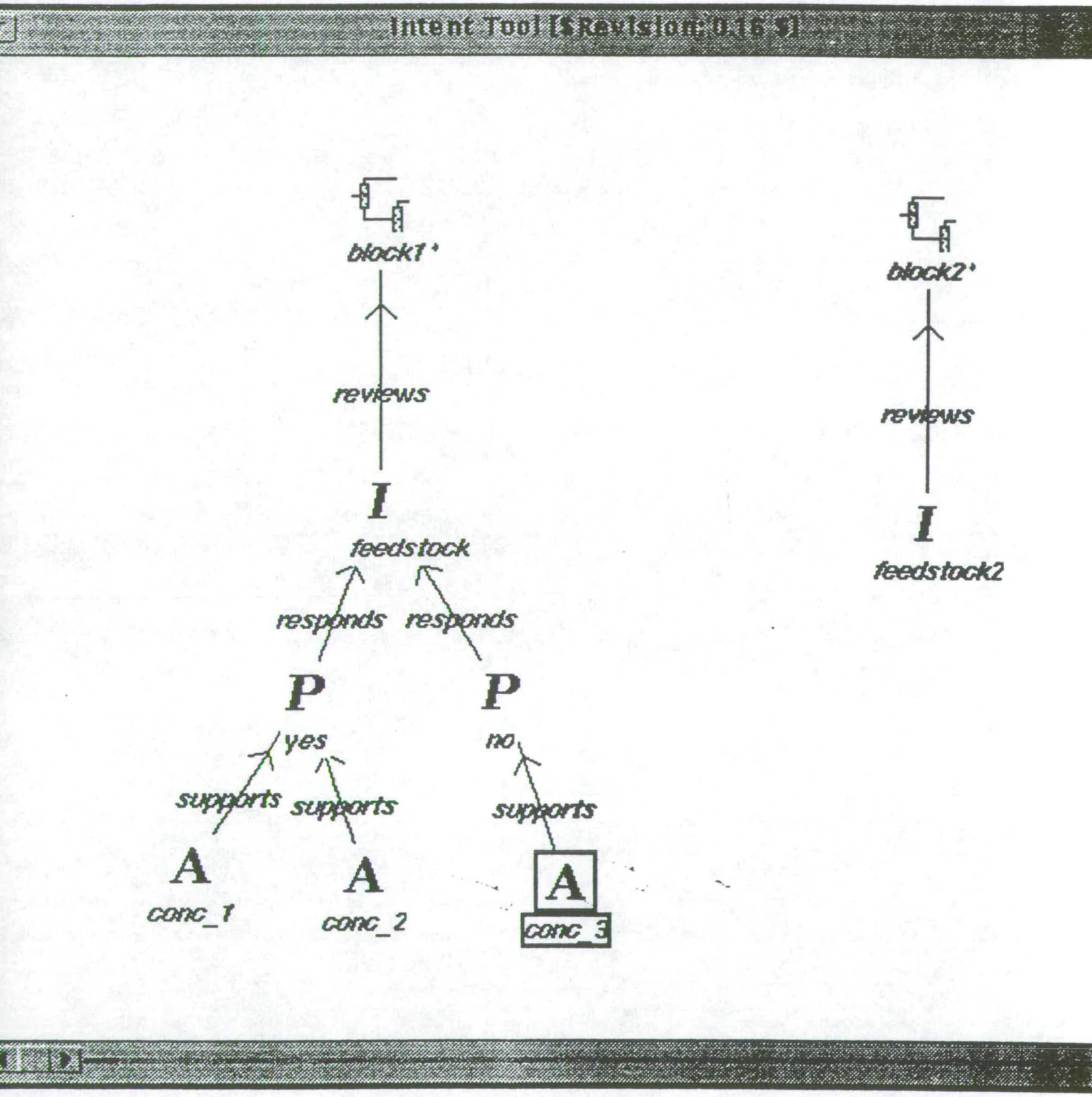
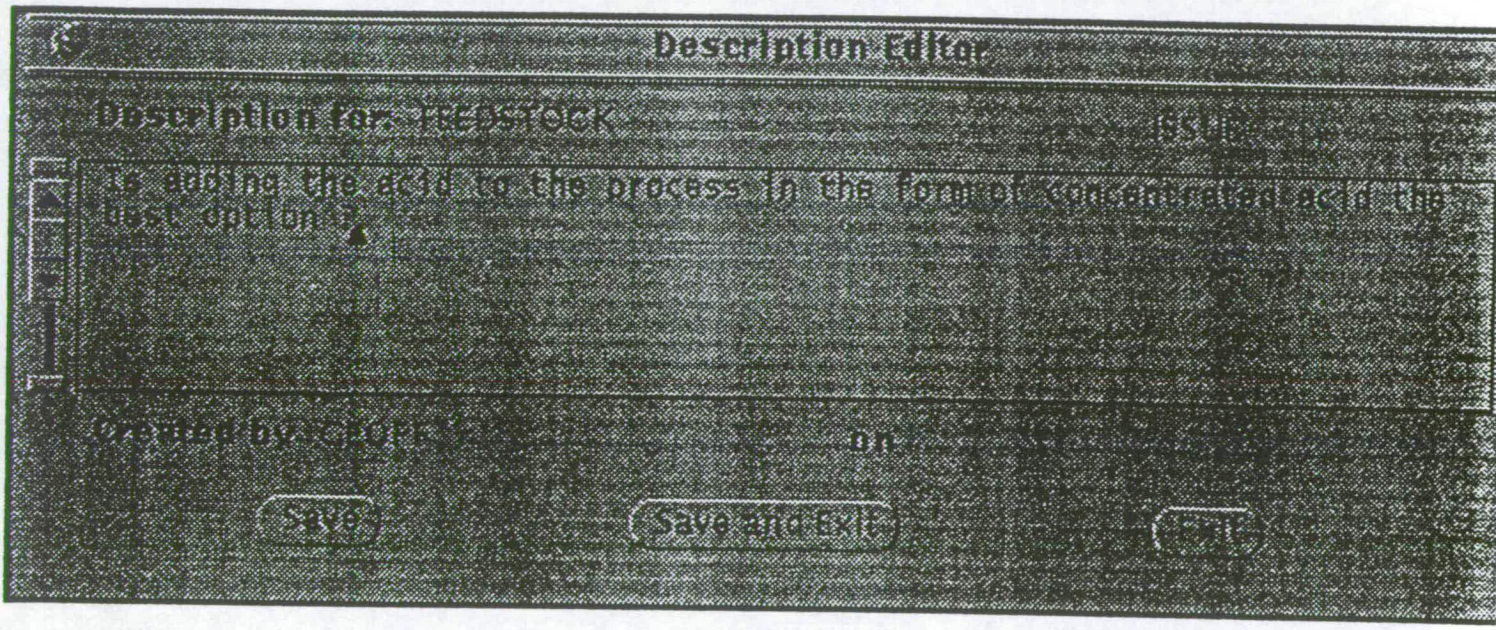

Intent Tool [$Revision: 0.16 $]
block1*
reviews
I
feedstock
responds
responds
P
P
yes
no
supports
supports
supports
A
A
A
conc_1
conc_2
conc_3
block2*
reviews
I
feedstock2

FIGURE 13


Description Editor
Description for: FEEDSTOCK
ISSUE
to adding the acid to the process in the form of concentrated acid the best option is
Created by: CHOPE
on:
Save
Save and Exit
Exit

Chapter 7

Use of épée

7.1 Introduction

During the lifetime of a process plant design large quantities of data are generated in many different formats and from many different sources. To handle this data effectively it is necessary to have a model of the data handling requirements. For the process industries the development of such a model was one of the objectives of the PISTEP initiative, discussed in Chapter 2, which resulted in the generation of an application protocol for process plant. Once a suitable model is available the necessary database can be established. Databases can be split into two groups depending on their architecture; relational and object-orientated. Relational databases are good for handling relatively simple relationships between data items presented in tabular form but have difficulty with more complex, graphical data such as that commonly encountered in the process industries, (Sawyer 1992). Object-oriented databases have been developed to address this issue. Rather than a strict segregation between programmes and data, an object can encapsulate both. This makes development, use, re-use, maintenance and modification of software easier as well as allowing movement between environments.

An appreciation of the importance of data management during the design process can be gained if the pattern of time usage by those undertaking design is considered. The results of a study into how the design engineers employed by an operating company spent their time undertaken with a view to determining why insufficient time was available to allow design optimisation are as follows, (Berzins and Jones 1989):

Engineering	24 %
Routine Paperwork	21 %
Data Gathering	19 %
Meetings and Travel	19 %
Immediate Items	10 %
Other	7 %

These figures represent average responses in each category with the range for engineering being between 10 and 35 %. It has been claimed, (Sawyer 1991), that process engineers can spend as much as 70 % of their time on information handling, representing nearly 10 % of total project cost for a contracting organisation. The reduction in lifetime asset cost of better data management has been given a minimum figure of 10 % by the PISTEP initiative with values up to 25 % possible, (Gardner 1995). The authors personal experience of working in a design environment indicates a reduction in emphasis on routine paperwork but a higher commitment to immediate items. This last item is particularly onerous if working in a task force environment where you are continually on hand to be approached with queries as they occur to people. Whilst this type of activity cannot be viewed as completely unproductive the interruptions to work patterns reduce the efficiency of time utilisation. During phases 1 and 2 of design the project team will be small and the structure less rigid than during the later phases, leading to an increase in the proportion of time available for engineering activities. Integrated tools must be able to support all design phases with usage of the facilities provided varying over time.

7.2 Data Exchange

Gutermuth views the requirements for integration from the stand point of an engineer within the process industry with limited access to computer resources and without the need for everyday usage, (Gutermuth 1992). He concludes that there are a number of areas in process engineering where standards for software design are required. The areas listed as important are physical property models, data inputting, report generation and data transfer between applications. The last of these is commonly acknowledged. One of the major obstacles to the integration of tools from a number of sources into an integrated environment has been the lack of any widely accepted standard for the exchange of data between the tools. The PISTEP initiative is aimed at addressing this point. A third generation demonstration tool has been produced and aims to show that all data is independent of the application that generated it and that all data can be accessed by any application, (Gardner 1995). This covered data from all phases of a project life, from conceptual design to decommissioning and demonstrated that information in a variety of forms could be

handled without any loss of attributes. Simply having a system of standard exchange protocols so that tools can talk to each other is not an end in itself as it does not take into account the handling of the data produced / used. The requirement for integrating STEP compliant tools are discussed by (Benayoune and McGreavy 1994).

7.3 Integrated Environments

To aid efficient working and help avoid the need to interface with a number of packages there is a wish amongst users of design tools that the different tools become integrated together. It has been pointed out, (Matzopoulos 1996), that the technology required to make this happen is, on the whole, already in existence and such systems have already been implemented on a small scale. The Windows operating system has features that can be exploited to provide the user with a workbench type system for process design, (Preece and Ingersoll 1990). Word processing, drafting, spreadsheeting and other tools are frequently provided within such a system but are not seamlessly integrated. Using "cut-and-paste" and being able to have a number of windows aids the user to swap information between applications within the environment. Windows based systems are a first step on the road towards integration.

Futterer mentions the need for an integrated system to ensure that process design can be carried out more efficiently, (Futterer 1972). The vision being to have seamless integration of chemical engineering calculations, specifications, cost optimization, mechanical design, drawing preparation, production of bid enquiries and production of operating instructions. For the time these were very sweeping aims and are still far from being realised. Futterer proposed a system called Process Compiler to start addressing the issues raised. This was essentially, viewed from the current position, a rather crude simulation tool with enhanced equipment sizing capabilities. Another early example is DIS (Design Integrated System) described by (Klemeś et al 1979). Using tools developed for the purpose, balancing, simulation and optimisation are included. Considerable effort was expended on communication with the system utilising a "fill-in-the-blanks" approach to inputting to assist, in particular, the infrequent user. This puts DIS ahead, in terms of user friendliness, of many systems that have followed it. At the same time Tsubaki and Motard

reported on the linking of a simulator, CHESS, to a database system, DPLS, as a first step towards an integrated environment, (Tsubaki and Motard 1979). Here considerable attention was paid to understanding the flow of information between the user and the computer and between computer tools. The focus was seen to be understanding how data becomes information and how information is used to make decisions. Without this understanding any tool developed will not be fully supportive of the project. Montagna and co workers also looked at linking a simulator and a DBMS but adopted a slightly different approach, (Montagna et al 1987). Here the focuses in developing SIMBAD were more efficient handling of data as user support and reducing the memory requirement for running a simulator. In SIMBAD, unit operation and physical property modules interact with the data base as independent programmes would, calling data when requested to undertake a calculation and returning the results to the data base when these have been completed. The memory required is thus limited by the largest module present. As dictated by this approach SIMBAD is based on a sequential modular simulator architecture. Leone and co workers report on the application of SIMBAD to the revamp of an iso-Propanol distillery, (Leone et al 1988), involving a high degree of non-ideality. Kam et al describe integration issues that arose during the development of a process evaluation system where the prime objective was to be user friendly and avoid exposing the user to the underlying database tool, dBase III, (Kam et al 1989). In addition to allowing the user to interact with the system via single key-strokes the software developed overcame problems of data communication between the different tools used. For an integrated environment to be of the greatest benefit to the user it is important that it is constructed with the needs of the user in mind. A key point in attempting to achieve this is to consider the amount of time spent on different activities during design. Whilst discussing the development of an integrated software package for the optimisation of multipurpose batch and semi-continuous plants, Shah and co workers give a list of requirements for an interface, (Shah et al 1995). These are listed below and would form a good basis for all interfaces.

(i) The interface must support the exploration of alternatives as well as data entry.

(ii) Access control and project management features must be included.

(iii) The interface must aid the user to correctly specify the problem by providing guidance on the data needed and by minimising the opportunity for typing errors.

(iv) The graphical representation of results should be adopted whenever possible to aid understanding.

A key aspect, not highlighted above, is the provision of adequate on screen help for users to guide them through the facilities available and how to use them. An alternative view of the future of integrated environments, based on the ASCEND language, is presented by (Westerberg et al 1989). The focus is the provision of a support system to integrate people, information and tools based on the principle that design is a social process. Under pinning the system provided is a clear understanding and model of the design process.

Early work in exploring the benefits and requirements of an integrated computer system for process plant design is described by (Winter and Newell 1977). The advantages of computer-aided design that are enhanced by an integrated environment are listed as:

Shorter design time scales

Better product

Lower operating costs

Lower investment

Lower design costs

A more reliable plant

The integration of data handling allowing one programme to accept as input the output of another, is quoted as a major contributor to the reduction in design time scale as well as reducing transcription errors. Winter and Newell emphasise the need to understand the process to be integrated before usable, supportive tools can be developed and discuss the results of a study to establish this information. These reinforce the criticality of data flow in an integrated system. The structure proposed by Winter and Newell relies on building links between applications. Motard discusses the requirements of a DBMS for enhancing process design by integration

of the disparate parts, (Motard 1989). The database structure is seen as key, moving from a relational data model towards an object-oriented approach to handle the diversity and complexity of the data encountered.

Sawyer describes an early attempt at an integrated environment aimed at introducing students to the concept of working under such conditions, (Sawyer 1988). The environment was very much constrained by the available hardware and software. The system, running under DOS and limited to 640 kB of memory, incorporated a steady-state simulator (CHEMCAD), a dynamic modelling tool (ISIM), a calculation spreadsheet (Lotus 1-2-3), a CAD package (AutoCAD) and a word processing package (Wordstar). CHEMCAD results were saved as ASCII files and imported into Lotus 1-2-3 spreadsheets to allow equipment design. Spreadsheet results were then imported into ISIM for dynamic simulation. The graphics output from CHEMCAD was saved in the DXF format and imported into AutoCAD to allow the preparation of engineering drawings. Whilst the system contained the required elements of an integrated environment it was far from seamless. Advances in data exchange and computing capabilities now allow much more elegant solutions to be adopted. McGreavy and Jiang describe an integrated environment, making extensive use of graphics for visualisation, for the distillation sub-problem, (McGreavy and Jiang 1996). The prime objective during development was the provision of a design support environment capable of handling concurrent design activities, for consideration of constraints such as safety, waste minimisation and flexibility, and providing greater insight into the consequences of design decisions. Using graphics-based presentation of data fits with the adage that "one picture is worth ten thousand words". The ability to "see" the impact of design and operating factors provides the insight into the problem. No case study work is described in any detail but such an approach shows a promising move towards the inclusion of the design factors, discussed in Section 4.2.3, from the earliest phases of a design. Also in the separation area Wahnschafft and co workers report on the integration of a synthesis tool, SPLIT, with ASPEN and an optimisation tool, (Wahnschafft et al 1991).

The concept of concurrent process engineering was developed to allow the life-cycle of a process to be considered during the early phases of design. This requires the cooperation and integration of the various discipline design activities that

take place. Integrated environments are attempts to implement concurrent engineering. The basic principles of data mapping and the use of multiple applications within a single environment are discussed by (Zhang et al 1996). Some implemented attempts at integrated environments are discussed below:

7.3.1 Aid Sim

Aid Sim was developed with the objective of assisting the user to carry out complex steady state simulations, (Alliet-Gaubert et al 1995). The structure is, similar to épée, designed to allow the linking of existing software including an existing simulator. Three aspects of simulation are supported by Aid Sim, preparation, results analysis and the use of multiple runs to gain an understanding of problem behaviour.

7.3.2 CHEIS

CHEIS (CHiyoda Engineering Information System) was developed by Chiyoda, a major Japanese contracting organisation, using DBMS techniques to integrate applications programmes for the design of refinery and petrochemical processes, (Niida et al 1977). The aim is to reduce the rework needed to transfer data between computer based design tools. Given the length of history implied by this the lack of success in general acceptance of this type of tool is disappointing. As no commercially available DBMS could be found to have all the characteristics identified as important by Chiyoda an in-house DBMS called CHEIS-OO was developed as a basis for the system. When considering the most appropriate way of using the DBMS Chiyoda considered writing applications programmes specific to it and slightly modifying existing programmes. The latter approach was adopted as it minimised the learning curve for users, allowed ease of revision incorporation and ensured that the application programmes are independent of the DBMS. Application programme managers were used to link programmes to the DBMS and had to be written for each interface to be included in the system. The applications were then invoked by commands given by the user. CHEIS was designed to support three design phases: firstly feasibility and case studies carried out on a number of single process units, secondly case studies on interrelated process units and finally more detailed design of a number of alternative process schemes.

7.3.3 Design++.

Design++ is described as an open-architecture Knowledge-Based Computer Aided Design (KB-CAD) tool which aims to support concurrent engineering and provide interfaces between various tools, (Tong and Sriram 1992). The tools included are CAD packages, relational databases, external engineering analysis packages and desk top publishing systems. Design++ thus extends conventional CAD drawing package abilities by allowing knowledge to be associated with objects. This ability allows, amongst other things, objects to carry information about their functionality, to include sizing routines and to maintain relationships. Such features coupled with access to external tools permits the CAD system to be used as a design tool. Tong and Sriram include an implementation of Design++ for the design of boiler systems. This was developed in Finland with the aim of improving the quality of design and decreasing the time taken. The implementation, IBPD (Integrated Boiler Plant Design), tackles the design of systems made up of fairly standard sub modules over the proposal, preliminary and detailed phases of design. It is not clear how much development time was required to produce IBPD and this could be an important factor for systems using less standardised sub assemblies. If suitable knowledge bases exist and do not have to be created then the open architecture of Design++ allows these to be added to the base system, thus reducing development time considerably. In principle, however, the approach could be extended to process plant design if all the appropriate elements and knowledge were included. When using IBPD as opposed to conventional design methods for the same type of problem, the design of recovery boiler air ducting, considerable savings are claimed: a calender time saving of 4.5 months and a designers time saving of 1,500 hours. Design++ uses AutoCAD as the main, tightly coupled, CAD package and it is not clear how easy it would be to include an alternative. The same comment applies to the relational database, design tools and publishing system.

7.3.4 DESIGN-KIT

DESIGN-KIT was developed by Stephanopoulos and co workers at MIT as a software support environment to aid process engineering, (Stephanpoulos et al 1987). A key instigating factor was a desire to see state of the art computing technology applied in the field of process engineering as it had been applied in other

engineering fields. Stephanopoulos and co workers describe the desirable attributes of support environments and discuss how DESIGN-KIT attempts to address these issues. Key factors identified and implemented within an object-oriented framework are as follows:

(i) Use of a graphical tool for the generation and manipulation of flowsheets, control structures etc. The window proposed for DESIGN-KIT is similar to currently available commercial graphical interfaces such as Model Manager for ASPEN.

(ii) The automatic generation of data structures describing the graphical objects. Attributes associated with object classes are utilised here.

(iii) Modular construction of objects and methodologies allowing an extremely flexible definition of the scope of the objects involved. The user can frequently define what constitutes an object.

(iv) Using high level description of tasks to aid user interaction but avoiding the need for each user to be familiar with the language used, LISP.

(v) Equation-oriented simulation. DESIGN-KIT is not designed to be a full simulator but the inclusion of manipulation of equation based systems was viewed as an essential design aid.

(vi) Reasoning capabilities to make full use of knowledge captured as production rules. This is used to support the design process and user driven synthesis. DESIGN-KIT does not function as an automatic synthesis tool.

(vii) Unified database management system to handle the quantity of information generated effectively.

No utilisation is made of software other than that designed for DESIGN-KIT, forcing any potential user away from tried and tested applications towards DESIGN - KIT applications that may not fulfil the same role. This is a result of DESIGN-KIT operating wholly within a Common-LISP based environment. Whilst yielding uniformity it reduces flexibility. An interesting feature of DESIGN-KIT is the inclusion of order-of-magnitude analysis for investigation of the effect of variation in design variables.

7.3.5 DesignMASTER.

DesignMASTER was jointly developed by ICI and ChemShare to achieve a step change in process design productivity by providing an integrated system of process tools, (Craft 1985). The user interface was with a menu driven central database acting as a front to design tools. The capabilities of these tools include simulation, equipment sizing, physical property prediction, drawing and specification sheet production. Productivity increases of 50 to 100% are claimed as the benefit of such a system, arising from the use of on screen prompting.

7.3.6 EDIT

Cassata and co workers describe the Engineering Design Integration Technology (EDIT) system developed by M.W. Kellogg to support their Fluid Catalytic Cracking Technology, (Cassata et al 1994). EDIT is made up of commercially available software: the interface component is MAGIC, the expert system shell ART-IM, the database ORACLE and the calculation engine ASPEN-plus. The platform utilised is a SUN Sparc server and workstations. The system contains design and operating data relating to FCCU technology and allows an engineer to either design a unit or rate the performance of an existing facility. EDIT is limited to a single technology with a relatively narrow scope of design and to become more general would require improvements to the information modelling capabilities. It does, however, provide an example of actual use of an integrated environment for design.

7.3.7 Engineering Toolkit

Shaw discusses work by SimSci to develop an engineering toolkit associated with a flowsheet simulator, (Shaw 1992). An object-oriented GUI based on a PFD representation is proposed to handle both the simulation and more detailed design calculations such as pump selection and line sizing. This appears to show a mismatch between the level of design implied by the representation, low, and that implied by the tools proposed, high. The simulator and other tools are separate but act on the same data base, with the latter generally operating in read-only mode. Example screens from the implementation are included by Shaw, these include the ability for the user to add tools into the system.

7.3.8 ICAS

ICAS (Integrated Computer Aided System) was designed to address the simultaneous design of processes and their control systems, (Gong et al 1995). It is a software environment that provides access to the various tools needed to carry out these activities. Central to the system is the simulator which has available a number of different solution strategies for steady state and dynamic simulation with or without controllers. The methodology used is set by the user process specification which also sets the forms of models to be used. Analysis features can also be accessed by the simulator allowing controllability and sensitivity aspects to be addressed. By allowing various forms of model (simplified, rigorous, reduced and linearized) and integrating steady state and dynamic simulations ICAS covers a number of project phases. Information can be passed directly between them. This is a key feature of integrated environments.

7.3.9 PEL

PEL (Process Engineering Library) is the ICI in-house suite of programmes to support all aspects of process design. Areas covered include hydraulics, physical properties, datasheets preparation and heat transfer, (Preston 1996). Preston describes how, over the period 1967 to 1987, PEL grew from half a dozen programmes used by a handful of engineers to over 80 programmes used by over 700 engineers worldwide. Key to this expansion was the move towards the use of VAX machines. The datasheet tool, PROVUE, was introduced in 1987 and Preston claims this as the first real process engineering database. The information contained within the database can be interrogated in a number of ways, for example to produce equipment lists, in addition to the production of datasheets. Revision control is a strong feature of PROVUE and is essential to ensure accountability. A history of the use of integrated environments within ICI is given by (Preston 1989). PEL does not function as an integrated environment but rather as a collection of useful process design tools available in one place. Interfacing, other than manual, between the tools does exist to a limited extent. For example HTFS heat exchanger design programmes can be run through PROVUE and the results imported directly into datasheets.

7.3.10 PROCEDE

The PROCEDE project based at the University of Leeds aimed to provide the engineer with a complete process design environment running on a desk top computer, (Preece and Stephens 1989). The underlying philosophy adopted was to ensure integration in a way that does not impose a particular way of working and to focus on the design process rather than on calculation procedures. This philosophy resulted in a proposed system which does not do any of the traditional design calculations but acts as graphical environment, interfacing and managing whatever applications the designer wishes to use. The use of a graphical environment allowed drawings and specification sheets to be prepared. Preece and Stephens point out that the degree of transparency involved in data management has a direct impact on the ability of the engineer to control the design process with complete transparency removing all control. To address this point the concept of modifiable transparency was built into PROCEDE allowing various modes of operation to be adopted. At one end of the scale all the information necessary to run an application could be assembled without any user actions and at the other the user would be required to input all this data. For integration the emphasis was on an open system using files or forms in the database to collect the information required by the applications whilst viewing the application packages as black boxes that are not altered in anyway. All necessary exchanges of information, between tools and the outside world are carried out by system tools whilst user tools provide the applications. PROCEDE was written in C and used a protocol for data transfer based on the Dynamic Data Exchange system within Microsoft Windows.

In 1995 a Windows based version of PROCEDE, version 2.1, capable of running on an IBM compatible PC became commercially available with an introductory price tag of £599, (Cherwell 1995). Thus the original project aim of developing a PC based tool has been realised, but it is highly questionable how complete the design environment is. The advantages and features highlighted throughout the sales literature are a reflection of the points that the software vendors consider to be the most significant. In the case of PROCEDE v2.1 the emphasis is on the ability of the programme to allow designers to manage data right through a project and to support the quick and easy preparation of presentation standard

drawings and specification sheets. At no point in any of the documentation is any mention made of the integration of application tools indicating a considerable shift in the aims of the commercial tool away from those described by Preece and Stephens when discussing the research tool. There is also no mention of the version for workstations using X Windows previously stated as a future development. The programme consists of four modules, described below.

FloSheet - An engineering drawing programme capable of supporting the generation of drawings ranging in complexity from sketches to P&IDs. Drawings can be imported or exported as DXF files with connection data as ASCII text files.

SymGen - A module for the management of a drawing symbol library. As well as providing a selection of standard symbols the capability to modify and add symbols is included.

SpecSht - Industry standard specification sheets are provided and linked with the graphical representation of the equipment on the drawing. Routines can be set up to import and export data.

SpecGen - A module for the management of the specification sheet forms. The standard sheets provided can be modified and new sheets created.

The ability to export files in formats that can then be used by other programmes goes a small part of the way towards integration but places the burden on the user rather than the design environment. As implemented, PROCEDE does not represent an integrated design environment although the underlying philosophy represents a significant move towards such a system.

7.3.11 PRODABAS

When first conceived PRODABAS was an attempt to use database technology to integrate design capabilities, (Angus and Winter 1985). It was written in FORTRAN 77 with the architecture of a relational database. The incorporation of existing tools into the system was acknowledged as important from the beginning of the design of the system. Interfaces with ASPEN PLUS, PROCESS and the HTFS programme TASC2 are reported. Additional application modules written specifically for PRODABAS are also included. The user interfaces with the system via an editor

that could support forms, reports, tables and graphics. PRODABAS was further developed by ASPEN as a multi-user system to integrate and exchange data between a number of calculation intensive programmes such as simulators, (Sawyer 1993). An application module interfaces to the programmes with applications operating on a proprietary database. This does not use the commonly occurring relational model. Integration and exchange within the PRODABAS environment is managed by the PDXI initiative.

7.4 Épée

Épée, an object oriented process engineering software environment, was developed in response to a need identified during the KBDS project, see Chapter 6, for an environment in which to carry out process design, (Ballinger et al 1994a). A major goal of the épée system is the sharing of data amongst a set of process engineering applications within a distributed environment, (Ballinger et al 1994b). It was recognised that all the standard tools should be available within this environment and that there should be no need to reinvent tools that already exist. Custom making tools to suit the environment would be a waste of effort. On examination the only tool found to be lacking was a general flowsheet editor and this was created within KBDS. It could be argued that the developing data exchange standards, see section 2.3.6, negate the need for an environment such as épée but the focus of the former tends to be on the exchange of detailed design information rather than the support of conceptual design. Presenting the user with a single GUI based system for interfacing to tools of all types aids ease of use as well as eliminating the need for repeated manual entry of data. Nothing implemented in épée precludes the use of any data exchange standard beyond the conceptual phase. Épée was originally conceived as an interface to a range of tools freeing the programmer from the need to write interfaces between programmes. The integration of KBDS and ASPEN into the épée environment is discussed by (Ballinger et al 1995).

The épée system is based on a client-server architecture with the server delegating work, managing databases and controlling the invoking of methods. Within the object oriented environment methods are applied to objects resulting in new objects. The methods are provided by applications, with some applications

providing a number of methods. Applications form the clients in the architecture and can be split into a number of categories. These categories are listed below, tools have been developed by the ECOSSE group at Edinburgh for the first five.

(i) Design environment applications such as KBDS.

(ii) Method providers such as CHiPS and PPDS.

(iii) Object browsers such as Obrowse.

(iv) Object editors such as DefComp and DefStream.

(v) Utilities such as unit of measurement editors and component databases.

(vi) Any third party applications that a user may wish to utilise.

The main function of Obrowse is to view and select objects from the database.

Spenceley and Ponton discuss the concepts behind the development of the épée GUIs, (Spenceley and Ponton 1995a). Rather than adopting a system oriented approach to GUI development épée followed an object oriented approach. Much commonly used engineering design software uses the former approach which enables the user to do a number of things within the environment. The major draw-back is that as the number of applications to be served increases the environment grows rapidly in size and can become uncontrollable. Without extensive training a user may be unable to negotiate a way through the resultant software or will only be able to utilise a small part of the available capabilities. Within épée objects are used to replicate design information used by an engineer and tools are applied to these objects. The GUI uses the objects as the visual key and supports the interaction with the tools. The épée GUI described by Spenceley and Ponton handles object editing on three conceptual levels:

(i) At the bottom level is data manipulation for entities that are best described as a numerical value eg pressure, diameter, product purity. This data can be assigned a status to indicate the reliance that can be placed upon it. The status combines with information on the origin of the value to form the basis of the épée data management system.

(ii) For more complex objects, such as streams, editing becomes more complex as different occurrences of the object type require a variety of treatments. The GUI must be able to support handling occurrences of the

same object type that appear in different contexts. For example with a stream the emphasis shifts depending on what the stream contains and the role it plays within the process. In one, the solids content could be vital and in another it could be the level of a contaminant.

(iii) When handling complex objects such as distillation columns and heat exchangers a graphical representation which can be directly manipulated forms the most user friendly depiction. This is commonly supported by flowsheeting tools. The direct manipulation of more basic objects is however not so commonly supported with most other direct manipulation environments being orientated towards documents. Épée aims to provide a more general object representation, as the document type may not always be applicable to process engineering, which can then be manipulated.

To avoid requiring users to remember how to use a number of different object editors épée adopts a house style for the GUIs.

Spenceley and co workers point out that one of the problems with using an object-oriented approach within an integrated process engineering environment is that there is no standard definition available for any given object, (Spenceley et al 1995b). This becomes a key issue when determining how data is to be passed between, and utilised by, a number of application tools. Épée addresses this point by using primary data within an object to define the type. Any data in excess of this can be added after the basic object has been created allowing the flexibility to accommodate multiple representations. The inheritance mechanism is then used to determine an objects identity and relationship to other objects. Object editors within épée have been developed to give a common interface to the objects and to access and edit the objects in a none specific way. Those implemented are DefComp, DefStream and DefGen. The first is a chemical component editor, the second a process stream editor and the last a generic editor aimed at object types that do not occur frequently enough to merit a dedicated editor. Other specific editors are planned.

Features of the épée object editors are as follows:

(i) The data entered can have a number of states reflecting the status, e.g. it

can be an approximation, fixed by the user or calculated by the system.

(ii) User input can be in virtually any units of measurement with automatic conversion to the selected base set.

(iii) Object transfer between editors and applications can take place via drag and drop.

(iv) Object data is shown in meaningful subsets such as heat and mass data.

(v) Object properties can be added or deleted.

In addition to an interface to a range of tools, épée can also be viewed as, (Ballinger et al 1994):

(i) A process oriented computer operating system.

(ii) A possible implementation and representation vehicle for parts of KBDS.

(iii) A generic technique for defining process engineering concepts.

The provision of object history and drag-and-drop features are key to the first of these. Implementing an object history allows the user to navigate through the large quantities of data generated during design with ease by providing information on the time, method and ancestry of each object. Drag-and-drop facilities ease the transfer of data between applications, e.g. PPDS physical property information into a stream or a mass balance into ASPEN. Currently the second of the above is served by the use of épée as a means of communication between KBDS and other applications. Épée allows KBDS users to view application programmes as transformation operators that can be applied to objects. For the third element épée aims to be a more convenient way for a programmer to communicate between two applications than by direct connection. The latter approach leads to the need for a large number of interfaces to be provided as the number of applications increases.

Épée provides an interface of three levels: object, message and transport. The object layer is concerned with the manipulation of objects, the message layer provides communication between the applications in the system in terms of épée objects and the message layer deals with the basic data transfer between distributed systems.

7.4.1 Test Case.

As it was know that CHiPS could not handle the HF case study, work on this

tool was based on the MEK case study.

When an épée run commences two windows are presented to the user, both open and one on top of the other, but work is not undertaken in either of these. The Obrowse window is the main user interface and is accessed via a command typed into a window opened using the normal background pull down menu. In comparison to KBDS it was not found to be easy to negotiate around épée, particularly at the start of a session, and these aspects would need to be considerable enhanced to aid the user. Difficulties in utilisation and a lack of links to other software tools meant that it was not found possible to undertake much case study work using this tool. The main views presented to the user are discussed in turn below.

7.4.1.1 Obrowse. The Obrowse window which appears when opening épée is shown in Figure 1. There are five pull down menus, File, Object, View, Methods and Properties, available at the top of this window, with the Methods menu also appearing if a right mouse button click is made in the working space. When objects have been entered into the system there are a number of different ways to display them, these are discussed below, but Figure 2 shows the most basic which does not provide any information or structure.

i) File. Contains the options Load Workspace, Save Workspace, Save Workspace as, Load Scratch Database, Load Database, Clear Browser, Print Window and About, all of which are self explanatory. A project to be brought into the system to be worked on can be brought in as a file or a database.

ii) Object. Contains the options Create New Object, Object Properties and Publish Objects. Choosing to create a new object brings up the Template Selector window, discussed below. With an item in the workspace highlighted selecting object properties brings up the Object Info window which gives the name of the object, how it was created, who created it, when it was created and the current status. Figure 3 gives an example for a component object.

iii) View. Contains the options View Object History, View Object Contents, View Object Structure, Hide Object, Show Ancestor, Show Descendants, Hide Ancestor and Hide Descendants. These allow the view of the workspace to be customised when choosing to display the objects in the history layout, selected from the properties menu.

iv) Methods. Contains the option Other Methods which has a sub-menu of Publish, Edit, View, Add and Apply Method. The last two of these are key elements in the use of épée. Selecting Add brings up the Select.Method window, Figure 4, which is discussed below. With on object highlighted using Apply Method brings up a window of that name which allows methods to be applied to the object. Figure 5 shows an example for a component object. The Add button on this window takes the user to the Select.Method window. Publish is used within épée to move items from the scratch database, where new objects are initially stored, into the published database. Objects within a scratch database can be quickly retrieved by the server but are difficult for other people to read. Scratch databases have a tendency to become rapidly cluttered with unimportant objects. Moving items into a published database allows housekeeping to take place and permits objects to be shared with other users.

v) Properties. Contains the options Browser and Object which allow the modification of the way in which the information contained within system is displayed to the user. The Object Info window is discussed above. The Browser Properties window has three forms, Figures 6, 7 and 8, selected from the pull down menu in the top left hand corner and each addressing a different aspect. In all cases depressing a button selects the alternative and causes it to be applied to the view. Figure 6 shows the most complex version, that addressing layout issues. Under layout there are four elements that can be altered, Label, Layout, Iconsize and a field specific to the layout chosen.

a) Label alters the amount of information displayed under each object and can vary from nothing, as in Figure 2, to everything available on the list. Neither of these extremes are very helpful to the user and it was found that using the alias as the label, as in Figure 9, was most useful. Using a combination of the date the object was created and the person who created it would be useful when considering design history.

b) Layout alters the arrangement of object icons. The simplest option is array where the icons are simply arranged, vertically or horizontally, in classes. Figure 2 is an example of this form which was not found to be useful due to the lack of structure. Selecting Contents gives a list of objects each with a

sub menu showing the slots that they contain, see Figure 10. The History option gives a structured view showing objects and methods applied to them to give new objects. This view, including alias labels, is shown in Figure 11 and was that preferred during testing. List gives a list of objects with as many labels as selected by the user, but there was a tendency for the data to exceed the width of the screen. Figure 12 shows an example. The Structure option was for viewing the contents of an object but is being replaced by View.Contents.

c) Iconsize. This simply gives four options for the size of the object icons. The largest was not found to be useful as the specific icons were lost and each object displayed with a common default. The choice between the other three would be purely down to the quantity of data the user wished to fit into the working space. The 32x32 options was found to be most useful during testing and is used in the print outs included.

Figure 7 shows the Browser Properties window in the Ordering form, this allows the order in which things are displayed to be modified. Alterations made there do not have any affect on the History view. Figure 8 shows the final form of the Browser Properties window, Limit View. This allows specific classes of objects to be removed from view and would be extremely useful when dealing with a large number of objects.

It could be said that there are too many options available to the user but in practise each person using the system would select their favourite style and stick to that, perhaps changing icon size as required by the complexity of the design.

7.4.1.2 Template Selector. As épée is an object oriented application, before methods can be applied an object has to be created. There were 59 options for template selection when creating a new object in the version tested. The Template Selector presents the user with a list of all the options available and gives information on the inheritance and slots contained within the template highlighted. Figures 13, 14 and 15 show this information for component, mixture and stream objects respectively. Once an object has been created it can be edited and have methods applied.

7.4.1.3 Select.Method. The basic Select.Method window is shown in Figure 4 and is one of the key elements of épée. The arrows by each item indicate the presence of sub menus.

i) Browse. An alternative route to the History, Objects and Structure browsers.

ii) Control. Gives access to the Unit Editor window, Figure 16, which allows the user to define the set of units they wish to work with and automatically converts between unit systems.

iii) Create. Gives access to the Create.Network window.

iv) Database. Commercial database tools Exodus and GDB are supported under épée. Various database functions are supported under this menu but were not used during testing.

v) Design. Provides a link to CHiPS for the design of separation sequences. These can be heat integrated, rigorous or simple. To be expanded to cover other method providers of this type.

vi) DumpObj. Allows an object to be dumped from the database.

vii) Edit. Gives access to the object editors, discussed below.

viii) GUI. Gives access to the Apply Method window.

ix) Physical_Property. Allows the user to select from a list of constant and variable physical property methods.

x) Select. This is an important option as it gives access to component selection window. Here the user can select components from the épée database that are to be used in the design. Figure 18 shows the Component Databank window used to select components. Other items that can be selected, by taking the user to the appropriate window, are applications, methods, slots and templates.

xi) Simulate. Gives access to ASPEN for the shortcut simulation of separation sequences.

xii) Synthesis. Provides the link to CHiPS for separation synthesis.

xiii) Vapour_Liquid_Equilibrium. Gives access to bubble point and dew point calculations.

xiv) View. Duplicates the options given under the Obrowse view menu but with the addition of a view of distillation profiles.

Links to both CHiPS and ASPEN did exist, but their use was found to be limited by the inability to adjust parameters within the models. The user should be presented with a list of default settings that have to be accepted or adjusted as necessary. The focus at the time of testing was also very much towards servicing only separation system design.

7.4.1.4 Slot Selector. The Slot Selector window contains a list of all the slots available within épée and allows them to be selected for addition to an object. Highlighting an item on the list displays information about the contents of the slot. Figure 17 shows an example for the Vapour-Heat-Of-Formation slot.

7.4.1.5 Object Editors. The component object editor initially used during testing, DefComp, has subsequently been modified but it is worth noting some comments on this tool. The means of adding components was found to be rather frustrating due to the quantity of information that had to be provided by the user. What is required is the ability for the user to state that a particular component is present and have all the associated information loaded from the physical property package being used, PPDS in this case, automatically. The modification of DefComp addressed these concerns by allowing a component to be selected and returned from a databank. Figure 19 shows the DefComp window.

In addition to the component editor stream, contents, generic object and mixture editors were available during testing.

7.4.1.6 Utilities. The épée units of measurement editor and components database were utilities used during testing. Having a reliable physical property method provider available is key to improving the productivity of process engineers by eliminating the need to spend time trawling through numerous paper sources to provide the necessary data.

7.4.2 Functionality.

The version of épée utilised was not found to be particularly useful when undertaking the test case. Difficulties with the object representation used by épée and in navigating around the structure were the main reasons for this failure.

In the contrast to the problems encountered with the loss of input to KBDS due to the saving routines, it was often found that épée saved too much information, in a rather unstructured way within the scratch database. This can be sorted out

when moving objects into a published database but this adds a step into the process which would be unnecessary if saving were more controlled. The tool was found to be very robust and difficult to crash, this should be viewed as an advantage but the indiscriminate saving of virtually all information should not be. Although there is a risk of gaps in design history it must be acknowledged that people make mistakes and change their minds and that consequently there should always be the option to select the data that is saved.

In the version of épée tested the functionality was restricted by the inability to create a stream from a set of components. Such a feature is necessary to allow the user to initially select all the components that are likely to be present and then use this pool to create streams.

7.5 Conclusions

The integration of the various design tools available is key to increasing the productivity of process engineers and reducing the occurrence of errors within the design process. To undertake an adequate test of the ability épée to undertake this role requires a more comprehensive and realistic trial than the one undertaken here. It is doubtful if a fair evaluation can ever be undertaken within an academic environment using a manufactured test case.

An integrated environment should allow the user to interface with all the tools needed during the design process via a single set of GUIs and permit all the disciplines involved in the design process to exchange information electronically. Whilst the automatic exchange of data between some tools may be desirable, for example line sizes from sizing calculations to P&IDs, to avoid an excessive level of change that could lead to confusion within a multiple user system it is more desirable that the user tells the system when information should be shared. The flagging of data status implemented in épée could be used to set access levels that would limit general availability of data until the originating discipline indicated that is was ready for release. Figure 20 lists the possible status settings within épée. If the data item subsequently changes control of the propagation of the change should be subjected to the same level of control. As well as access controls it is also necessary for an integrated system to include control over the methods that are applied by the users.

As a minimum this would be needed to ensure the consistency of tool revision.

FIGURE 1

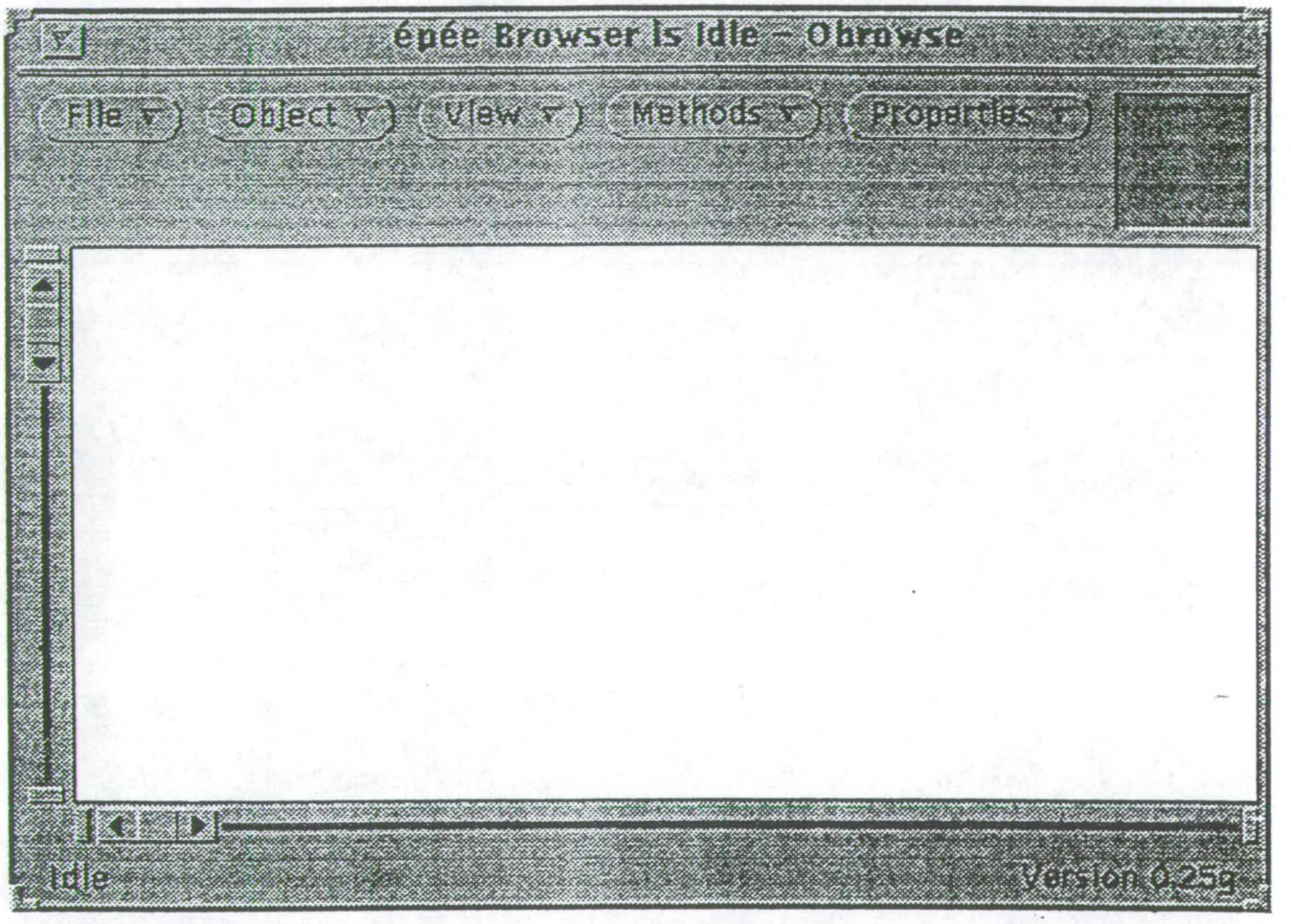

épée Browser Is Idle - Obrowse
File
Object
View
Methods
Properties
Idle
Version 0.25g

FIGURE 2

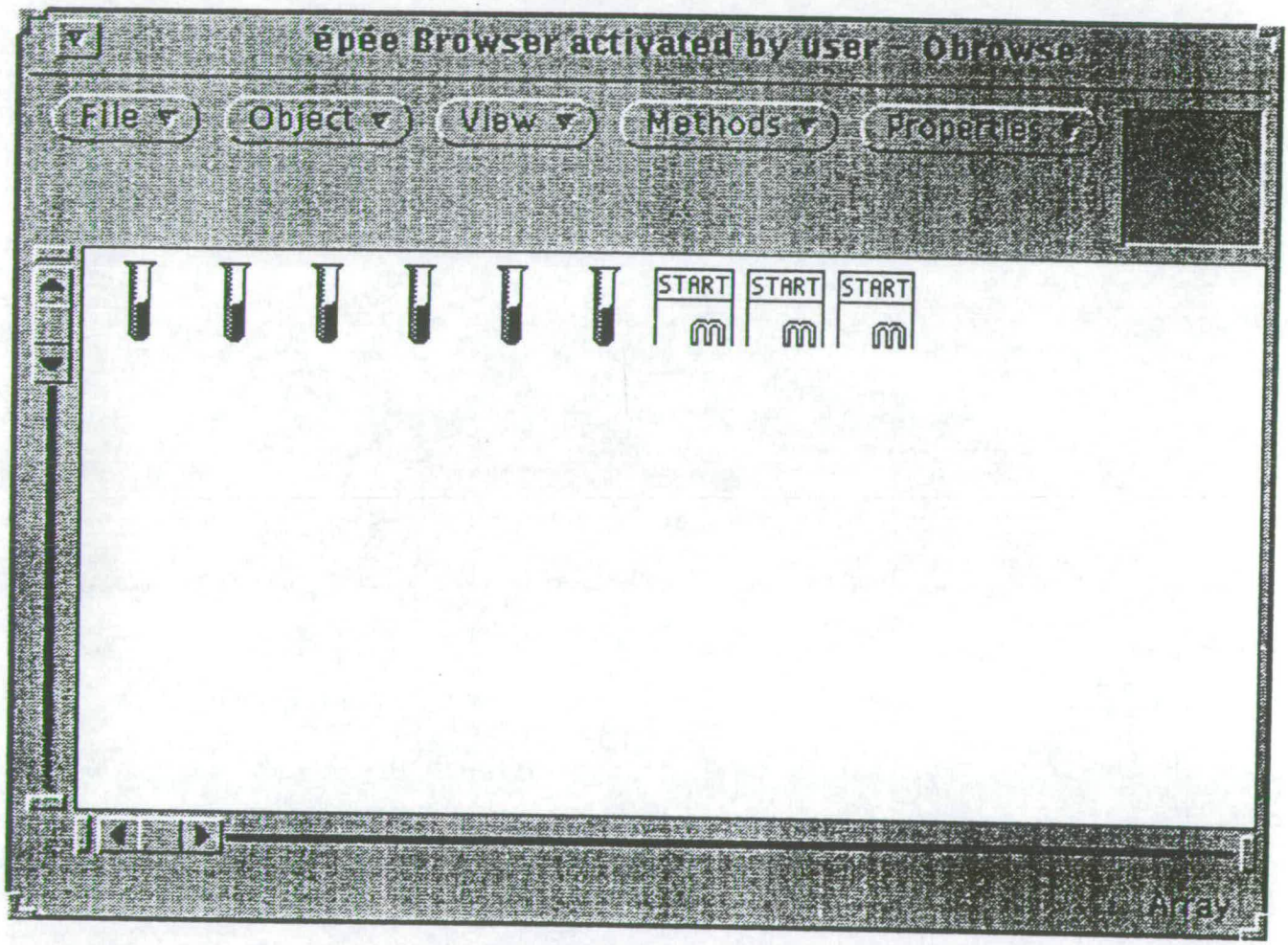

épée Browser activated by user - Obrowse
File
Object
View
Methods
Properties
START
START
START
Array

FIGURE 3

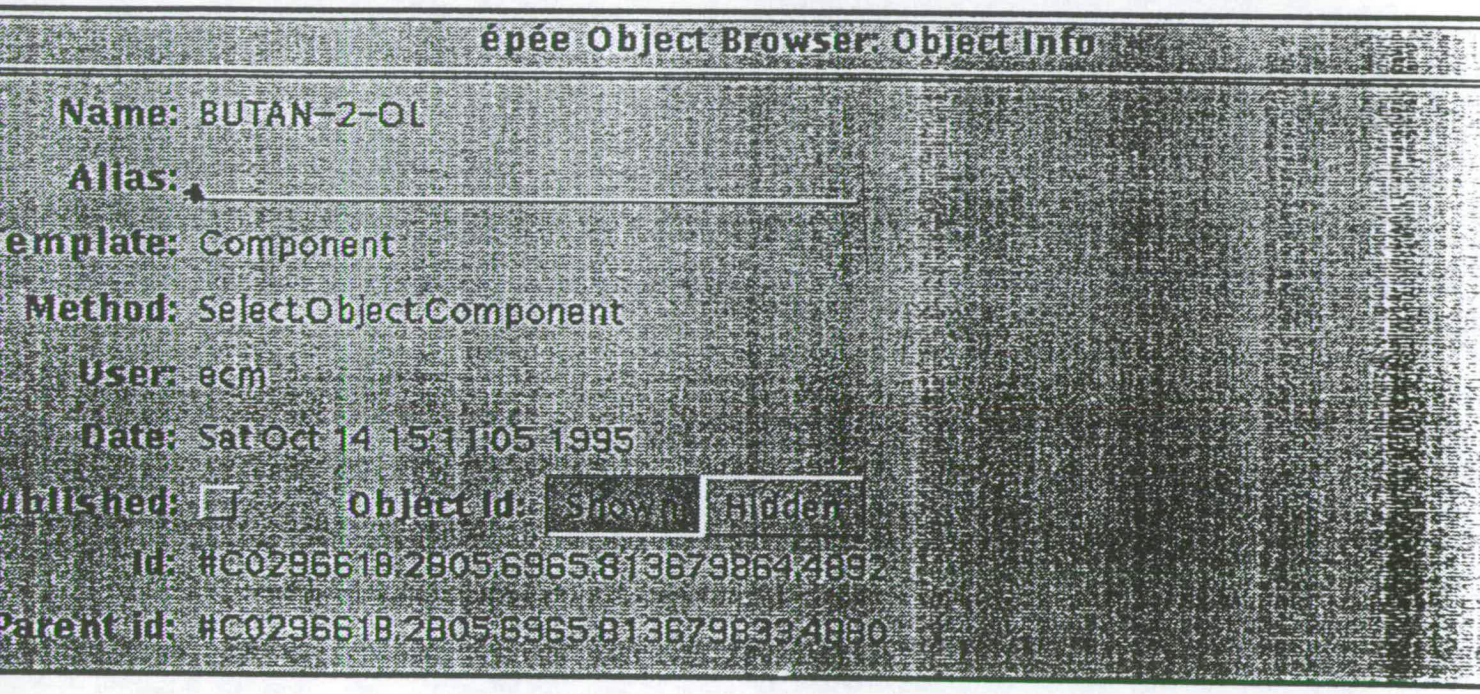

épée Object Browser: Object Info
Name: BUTAN-2-OL
Alias:
emplate: Component
Method: Select.Object.Component
User: ecm
Date: Sat Oct 14 15:11:05 1995
ublished:
Object Id:
Shown
Hidden
Id: #C029661B.2B05.6965.81367986.4892
Parent Id: #C029661B.2B05.6965.81367933.4BB0

FIGURE 4

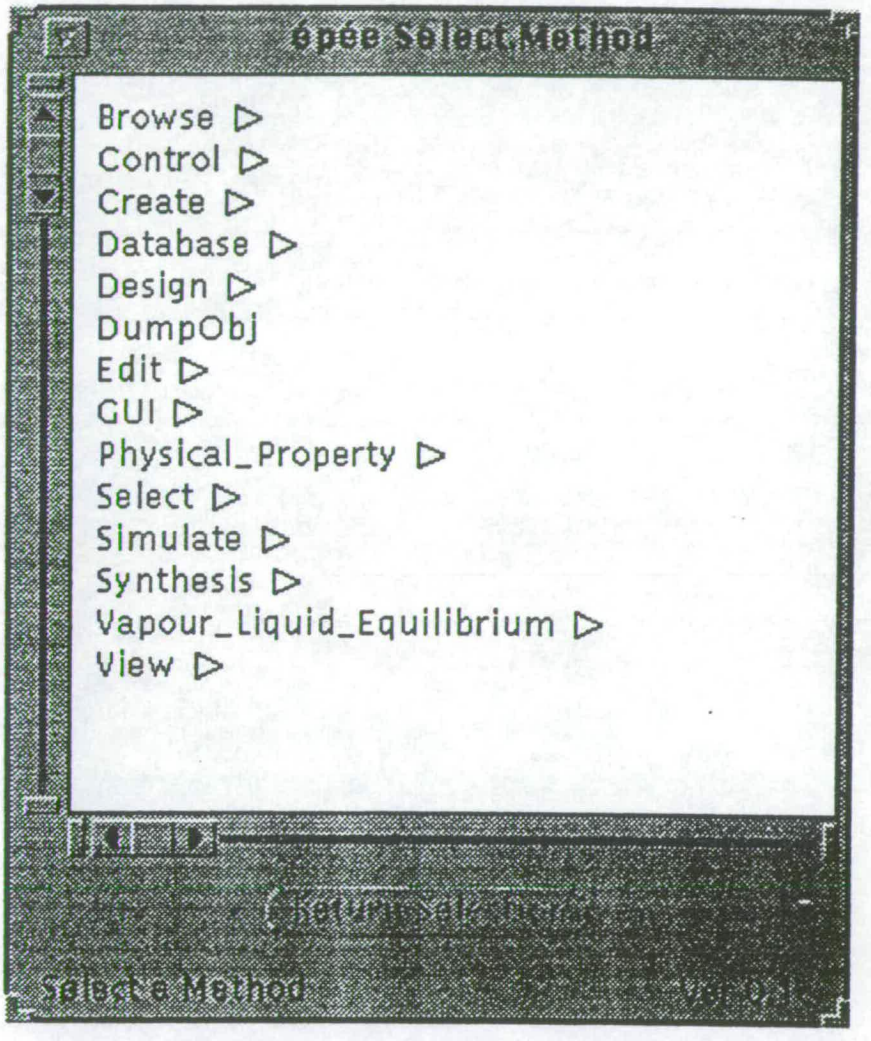

épée Select Method
Browse ▷
Control ▷
Create ▷
Database ▷
Design ▷
DumpObj
Edit ▷
GUI ▷
Physical_Property ▷
Select ▷
Simulate ▷
Synthesis ▷
Vapour_Liquid_Equilibrium ▷
View ▷
Select Method

FIGURE 5

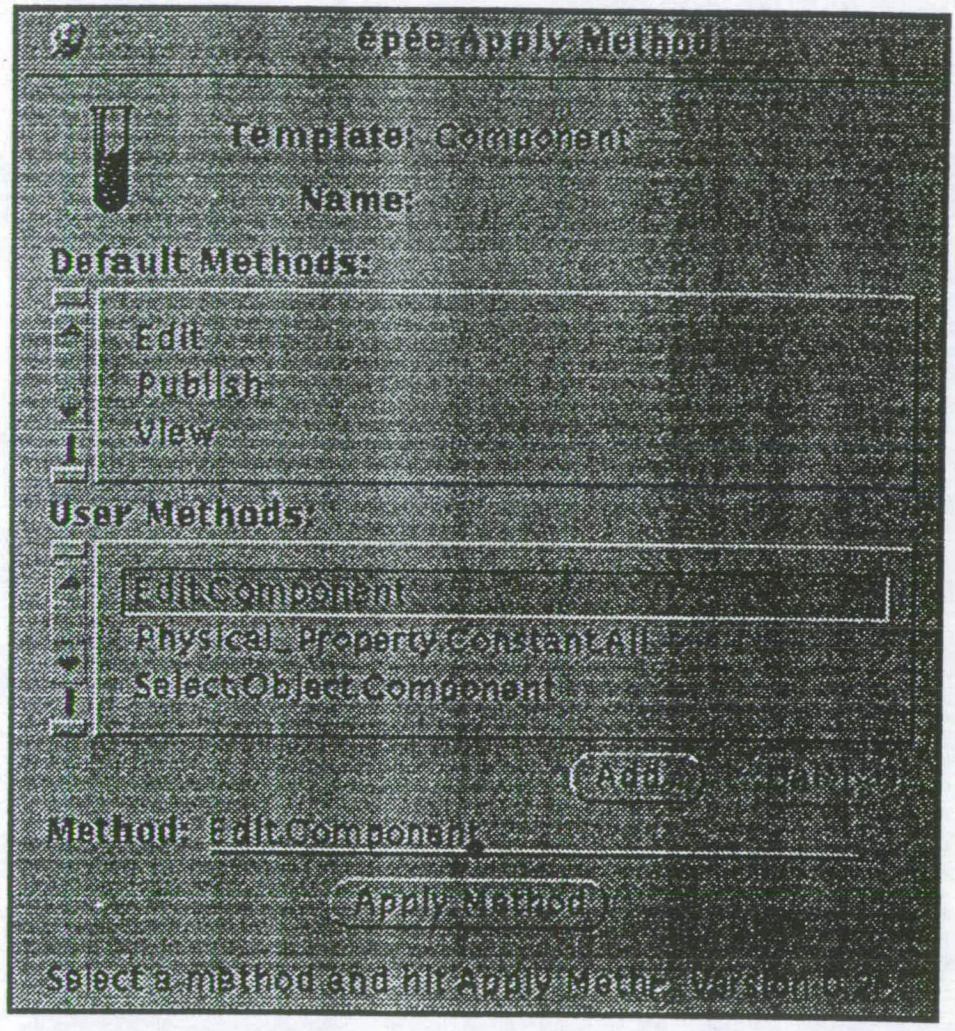

Epée Apply Method
Template: Component
Name:
Default Methods:
Edit
Publish
View
User Methods:
EditComponent
Physical_Property Constant All
SelectObjectComponent
Add
Method: EditComponent
Apply Method
Select a method and hit Apply Method

FIGURE 6

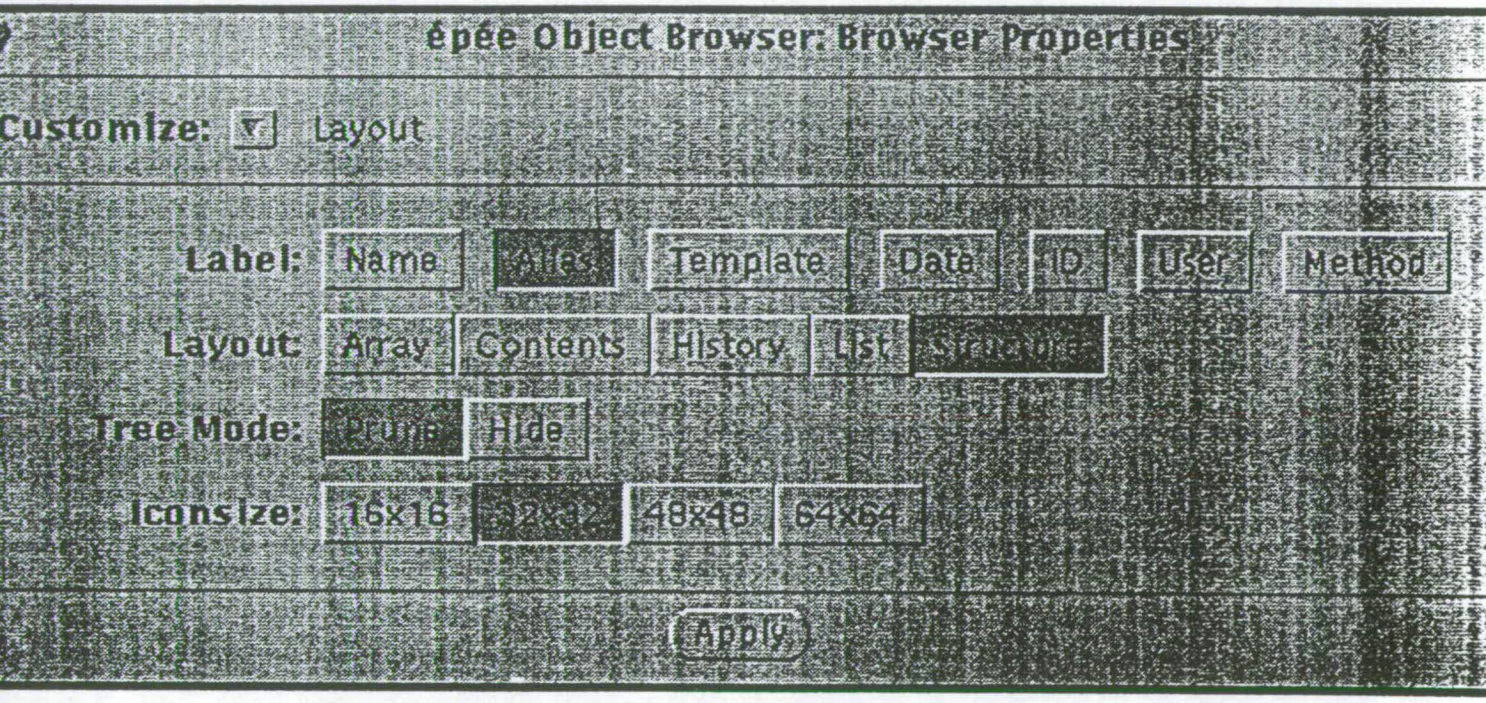

épée Object Browser: Browser Properties
Customize:
Layout
Label:
Name
Alias
Template
Date
ID
User
Method
Layout:
Array
Contents
History
List
Tree Mode:
Prune
Hide
Iconsize:
16x16
32x32
48x48
64x64
Apply

FIGURE 4

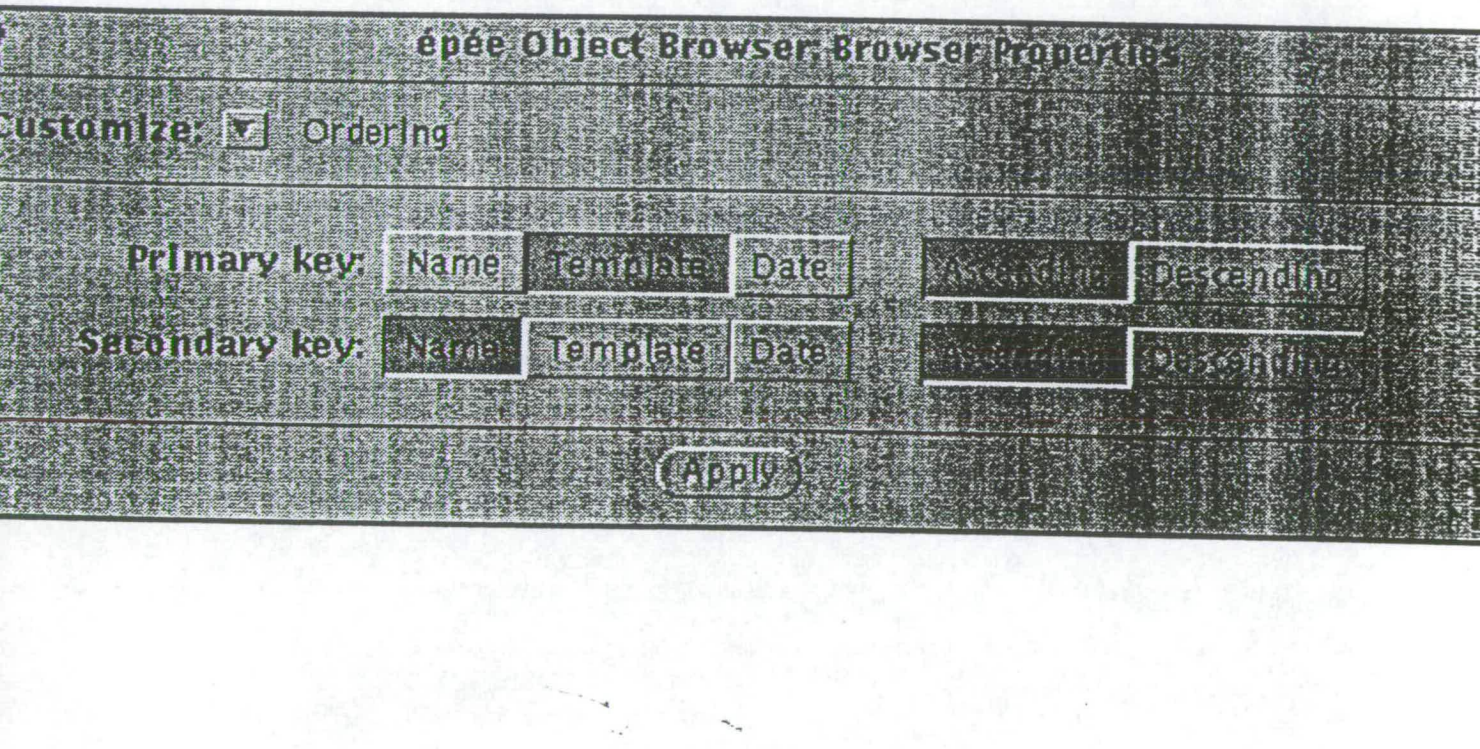

épée Object Browser Browser Properties
Customize: Ordering
Primary key:
Name
Template
Date
Ascending
Descending
Secondary key:
Name
Template
Date
Ascending
Descending
Apply

FIGURE 8

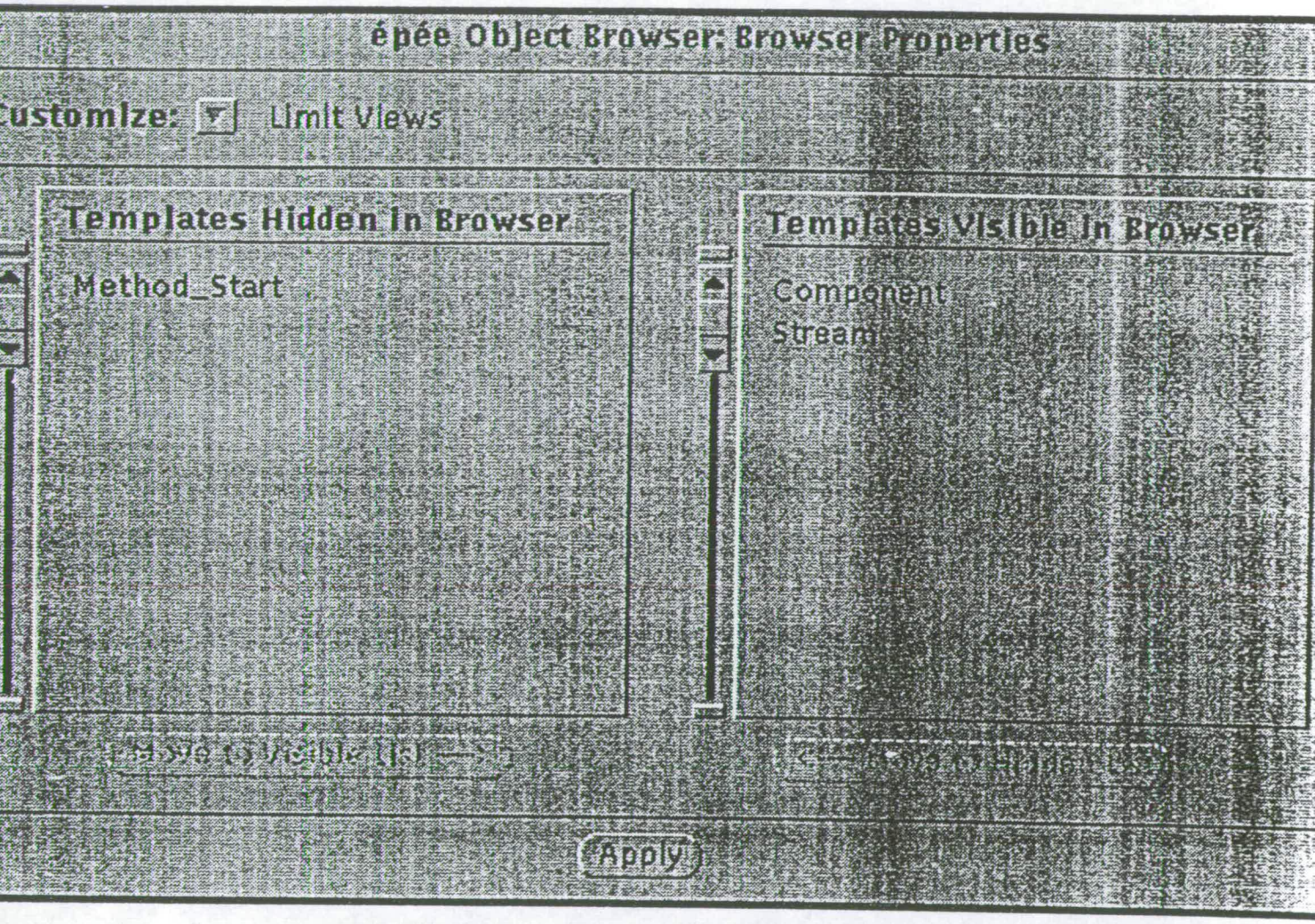

épée Object Browser: Browser Properties
Customize:
Limit Views
Templates Hidden In Browser
Method_Start
Templates Visible In Browser
Component
Stream
Apply

FIGURE 9

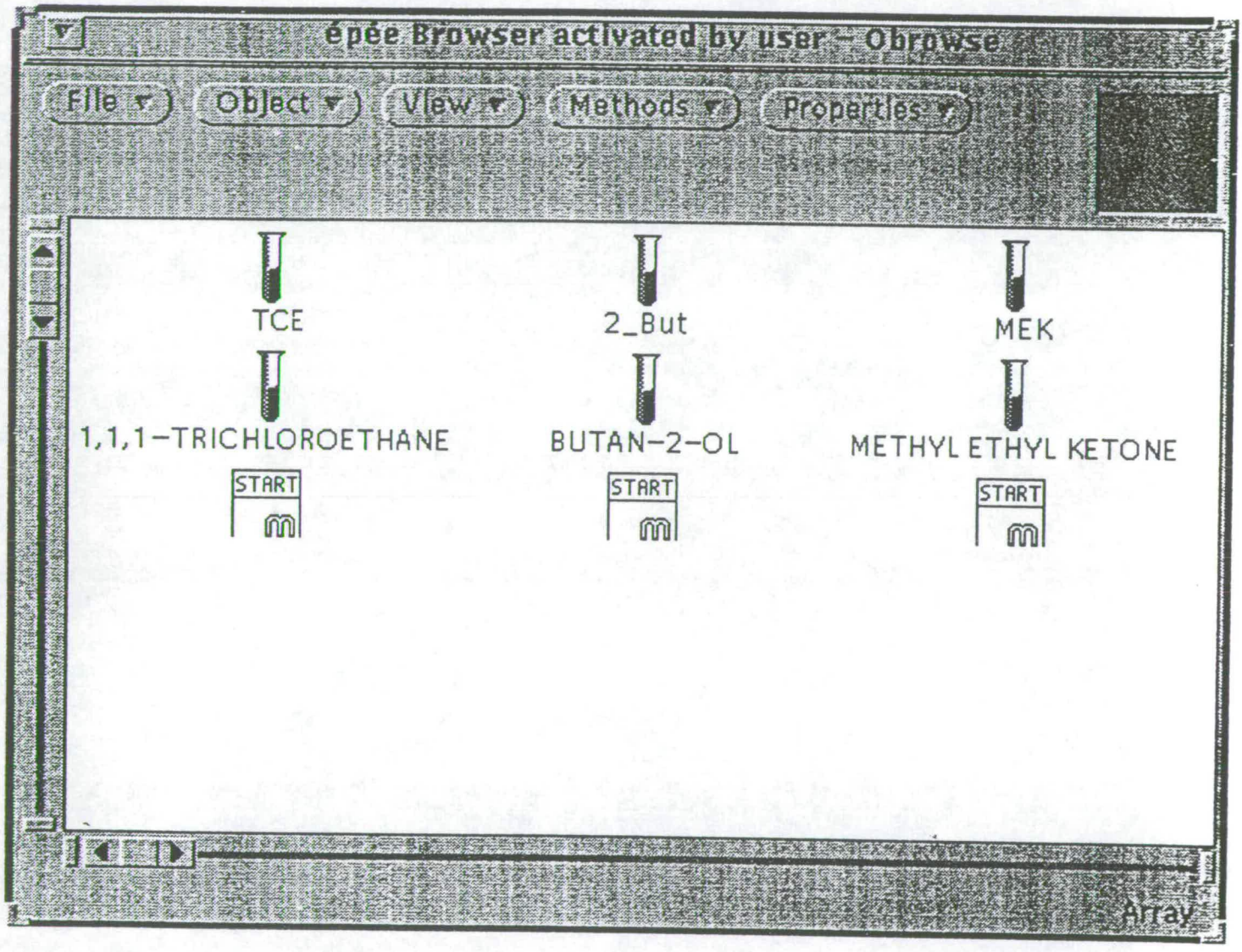

épée Browser activated by user – Obrowse
File
Object
View
Methods
Properties
TCE
2_But
MEK
1,1,1–TRICHLOROETHANE
BUTAN–2–OL
METHYL ETHYL KETONE
START
START
START
Array

FIGURE 10

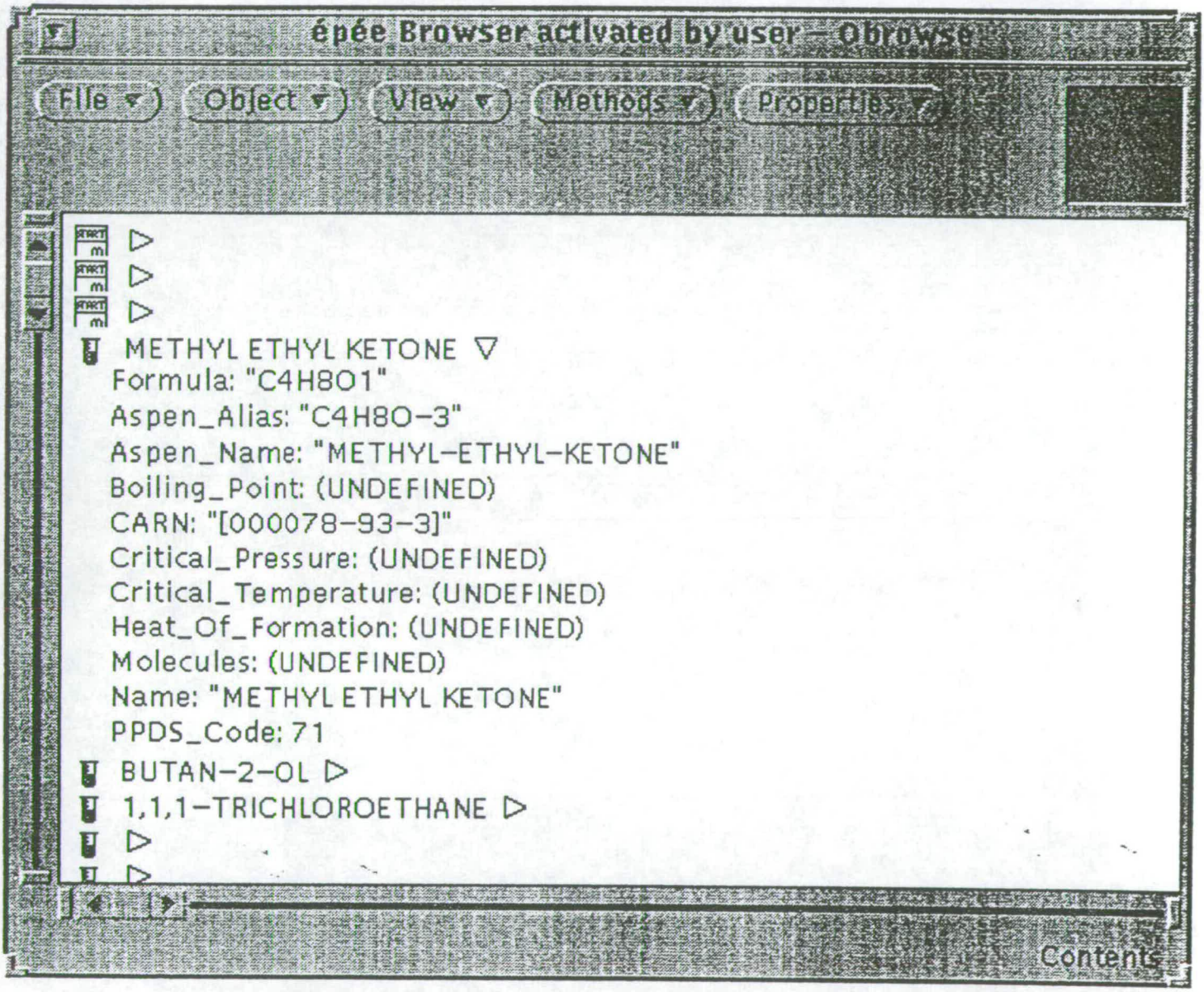

épée Browser activated by user – Obrowse
File
Object
View
Methods
Properties
METHYL ETHYL KETONE
Formula: "C4H8O1"
Aspen_Alias: "C4H8O-3"
Aspen_Name: "METHYL-ETHYL-KETONE"
Boiling_Point: (UNDEFINED)
CARN: "[000078-93-3]"
Critical_Pressure: (UNDEFINED)
Critical_Temperature: (UNDEFINED)
Heat_Of_Formation: (UNDEFINED)
Molecules: (UNDEFINED)
Name: "METHYL ETHYL KETONE"
PPDS_Code: 71
BUTAN-2-OL
1,1,1-TRICHLOROETHANE
Contents

FIGURE 11

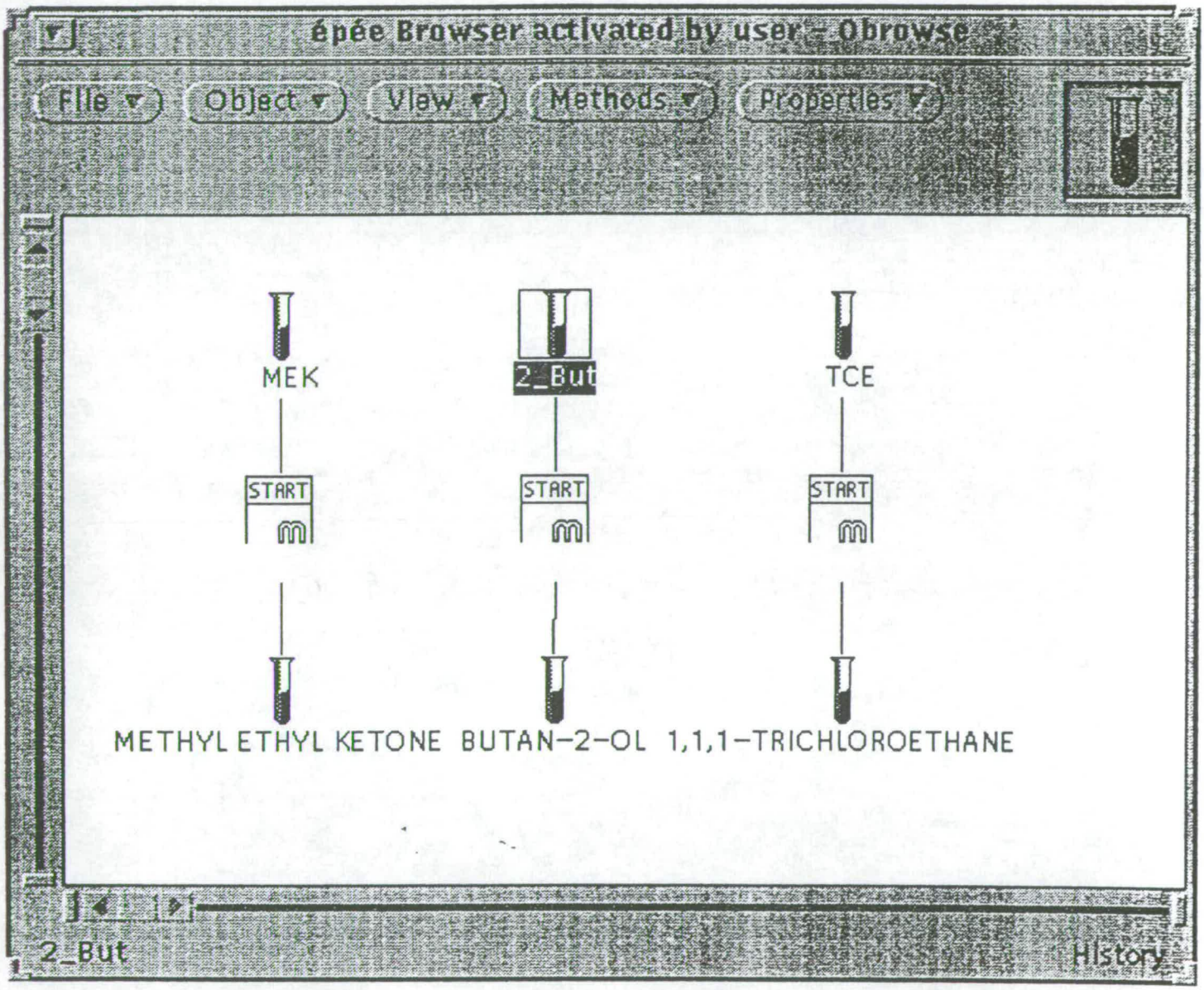

épée Browser activated by user - Obrowse
File
Object
View
Methods
Properties
MEK
2_But
TCE
START
START
START
METHYL ETHYL KETONE
BUTAN-2-OL
1,1,1-TRICHLOROETHANE
2_But
History

FIGURE 12

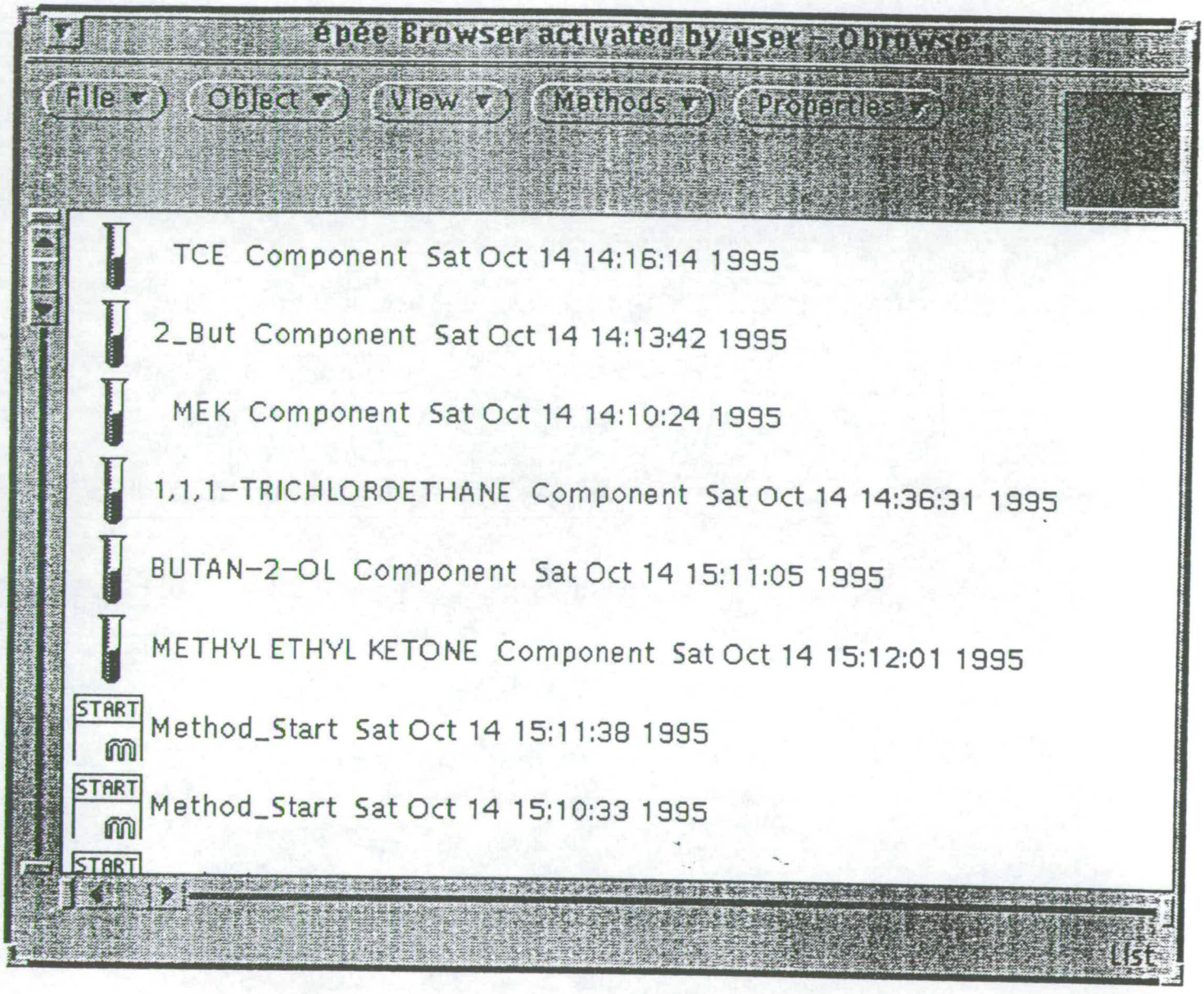

épée Browser actlvated by user - Obrowse
File
Object
View
Methods
Properties
TCE Component Sat Oct 14 14:16:14 1995
2_But Component Sat Oct 14 14:13:42 1995
MEK Component Sat Oct 14 14:10:24 1995
1,1,1-TRICHLOROETHANE Component Sat Oct 14 14:36:31 1995
BUTAN-2-OL Component Sat Oct 14 15:11:05 1995
METHYL ETHYL KETONE Component Sat Oct 14 15:12:01 1995
START
Method_Start Sat Oct 14 15:11:38 1995
START
Method_Start Sat Oct 14 15:10:33 1995
START
List

FIGURE 13

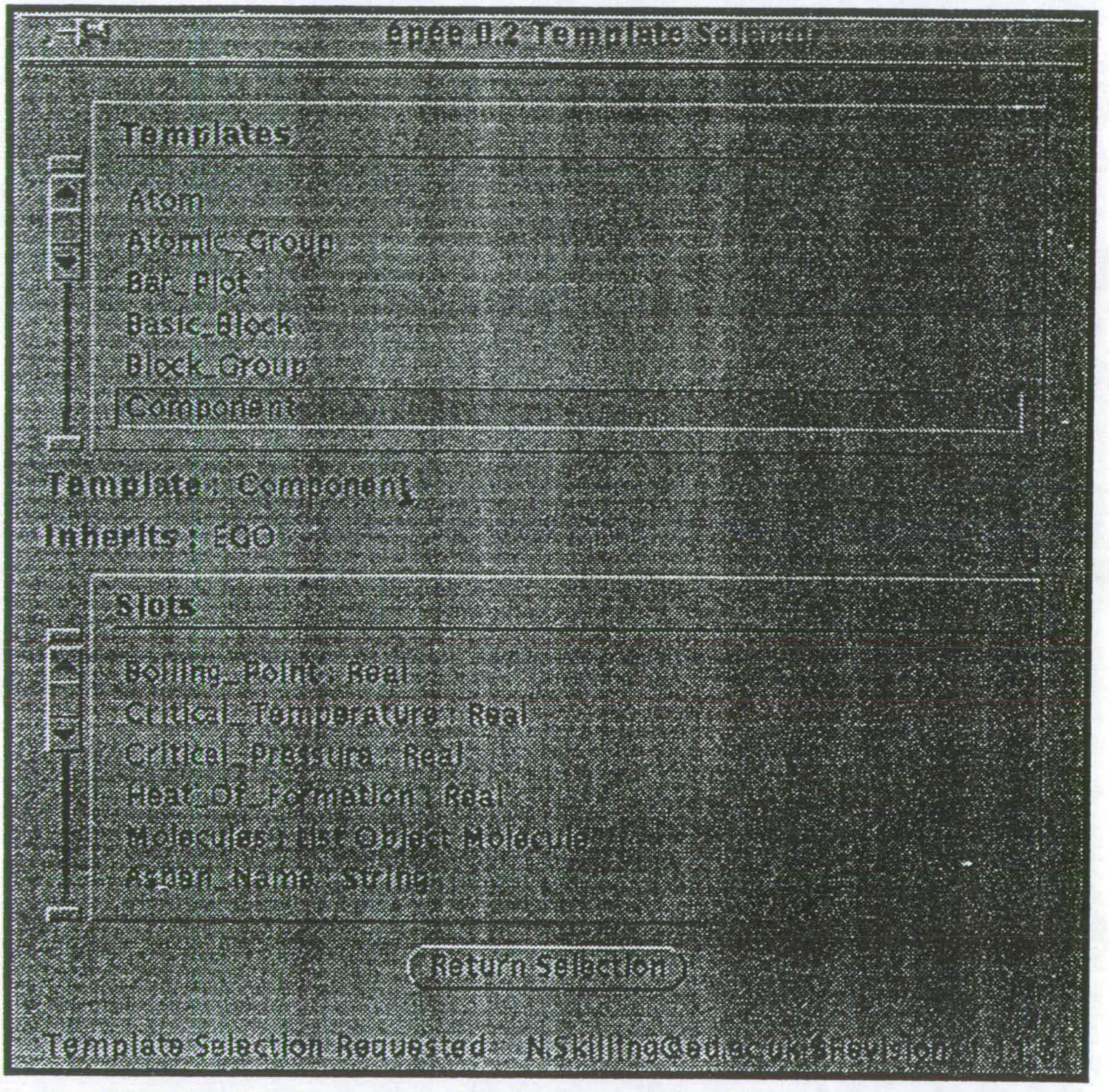

Templates
Atom
Atomic_Group
Bar_Plot
Basic_Block
Block_Group
Component
Template : Component;
Inherits : EGO
Slots
Boiling_Point : Real
Critical_Temperature : Real
Critical_Pressure : Real
Heat_Of_Formation : Real
Molecules : List Object Molecule
Atom_Name : String
Return Selection

FIGURE 14

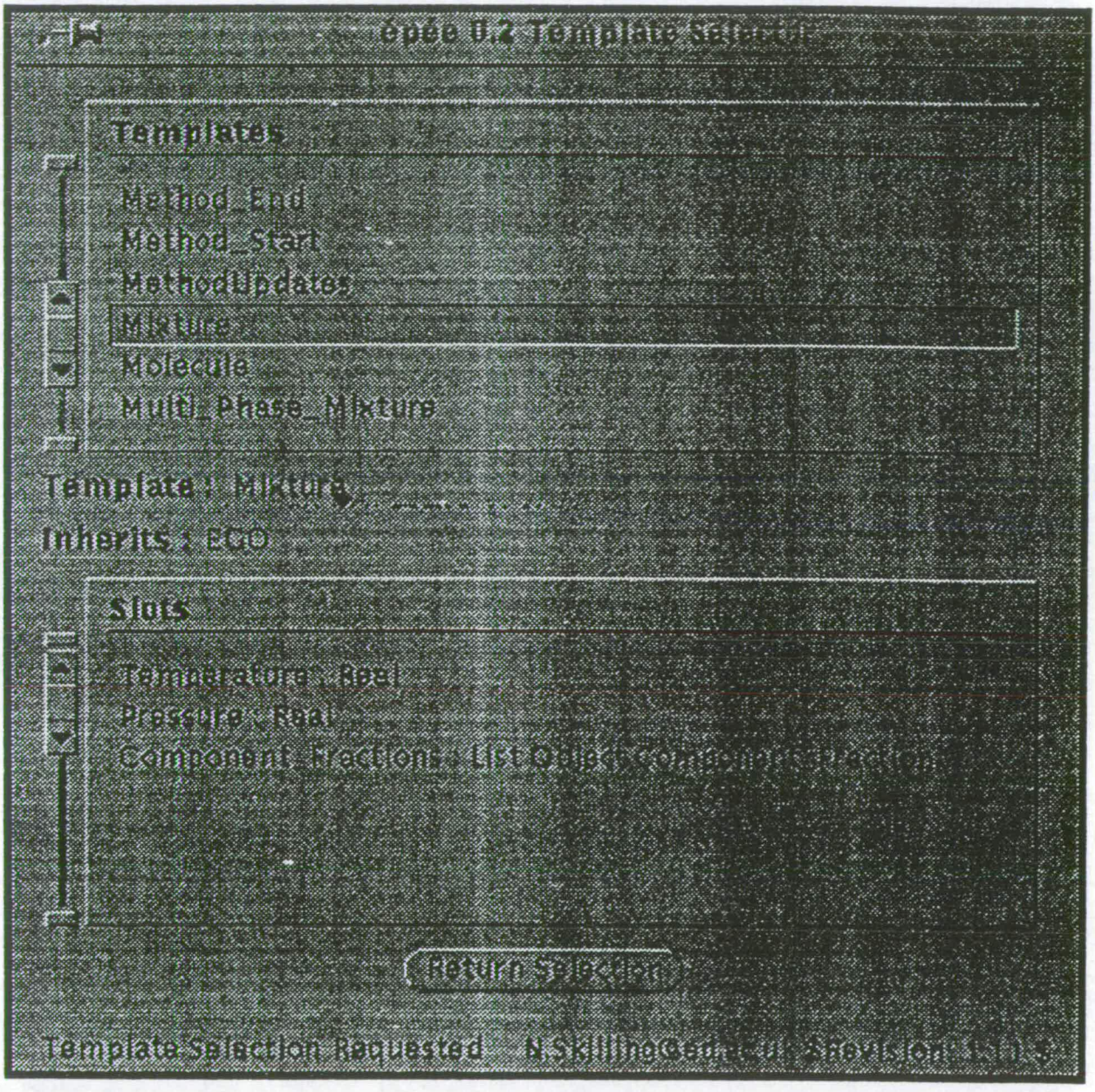

epée 0.2 Template Selector
Templates
Method_End
Method_Start
MethodUpdates
Mixture
Molecule
Multi_Phase_Mixture
Template : Mixture
Inherits : ECD
Slots
Temperature : Real
Pressure : Real
Component_Fractions : List Quick
Return Selection
Template Selection Requested

FIGURE 15

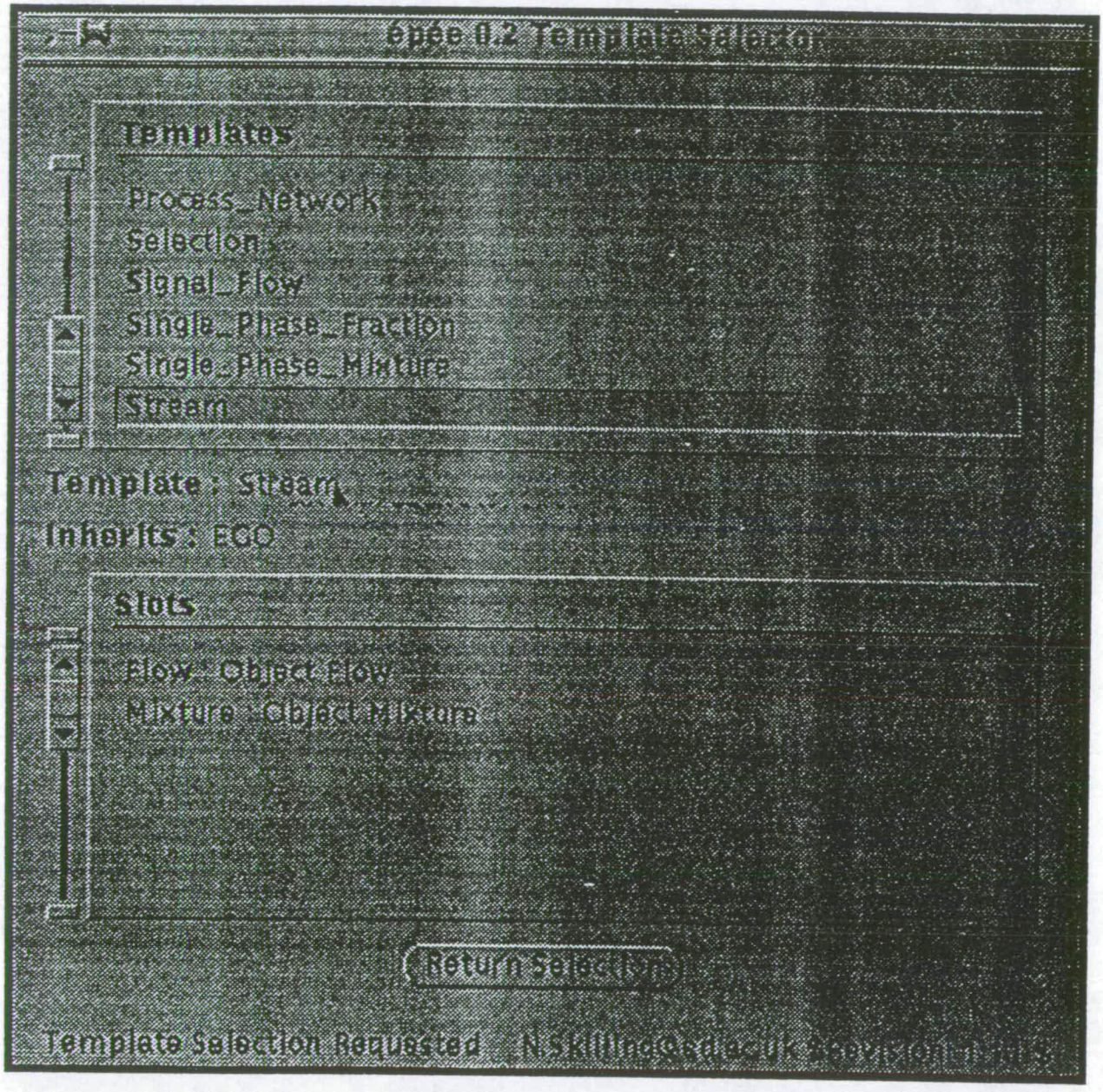

epee 0.2 Template Selector
Templates
Process_Network
Selection
Signal_Flow
Single_Phase_Fraction
Single_Phase_Mixture
Stream
Template : Stream
Inherits : ECO
Slots
Flow : Object Flow
Mixture : Object Mixture
Return Selection
Template Selection Requested

FIGURE 16.

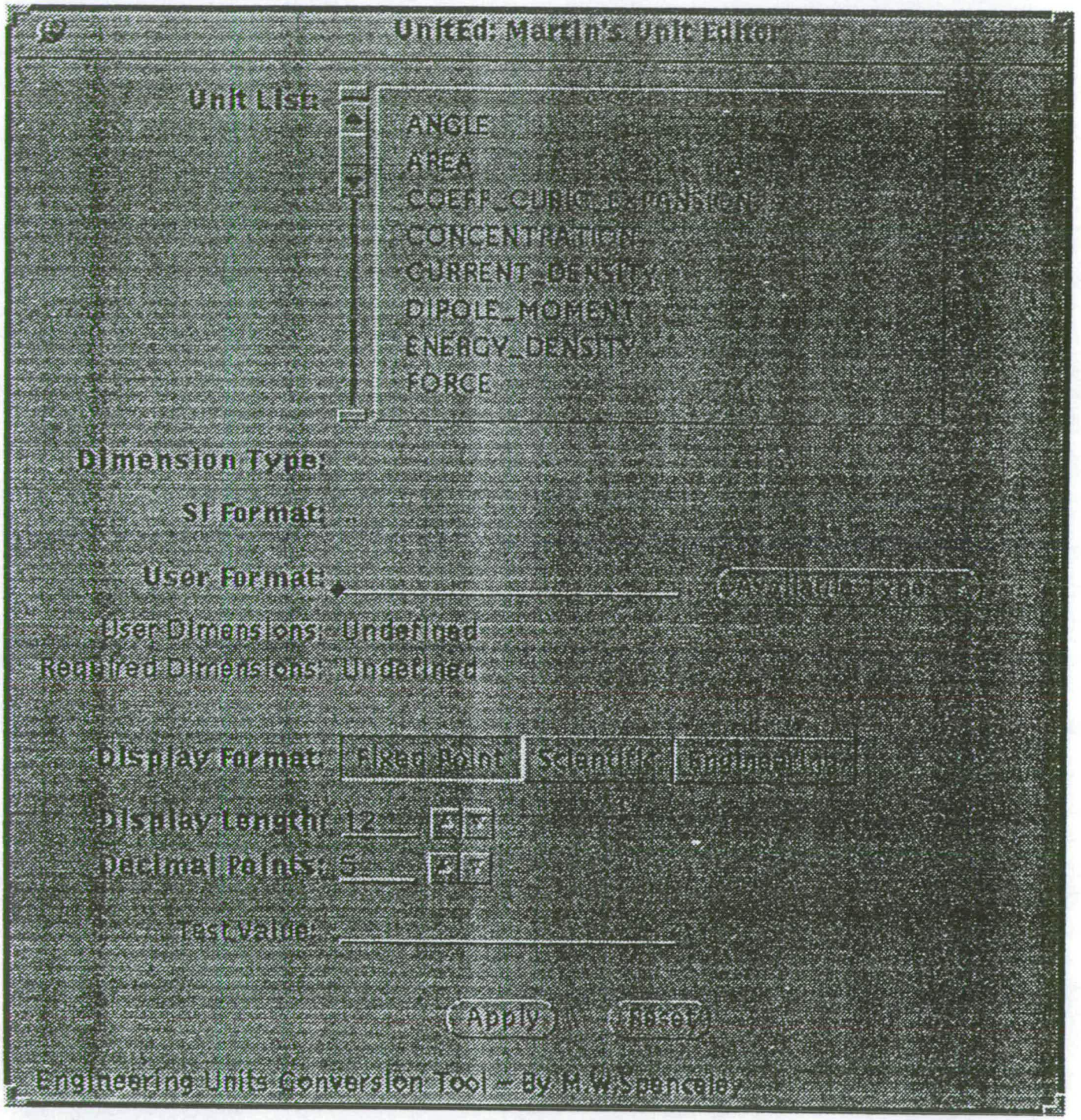

United: Martin's Unit Editor
Unit List:
ANGLE
AREA
CONCENTRATION
CURRENT_DENSITY
DIPOLE_MOMENT
ENERGY_DENSITY
FORCE
Dimension Type:
SI Format:
User Format:
User Dimensions: Undefined
Required Dimensions: Undefined
Display Format:
Fixed Point
Scientific
Display Length: 12
Decimal Points: 5
Test Value:
Apply
Reset
Engineering Units Conversion Tool -- By M.W.Spencely

FIGURE 17

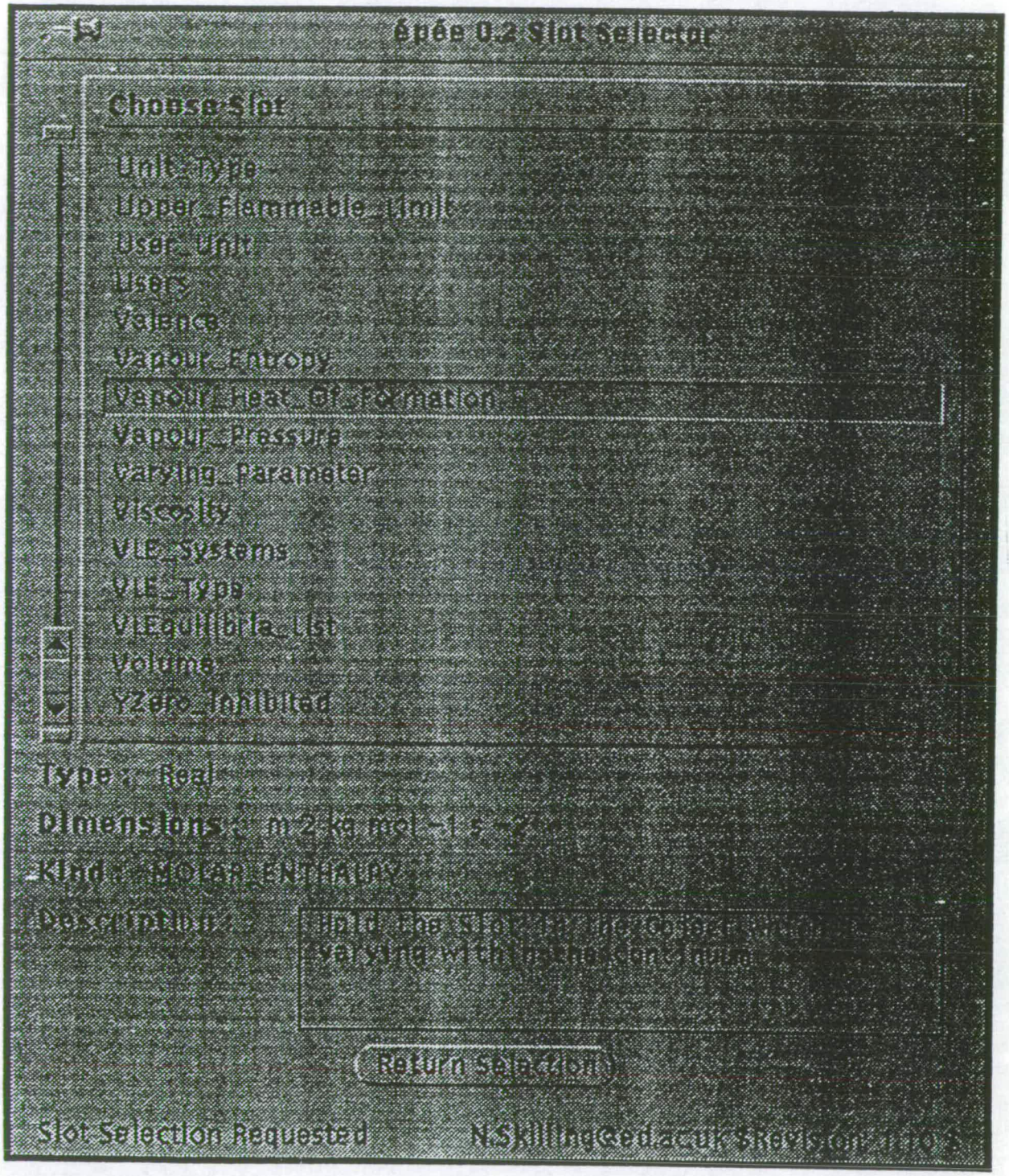
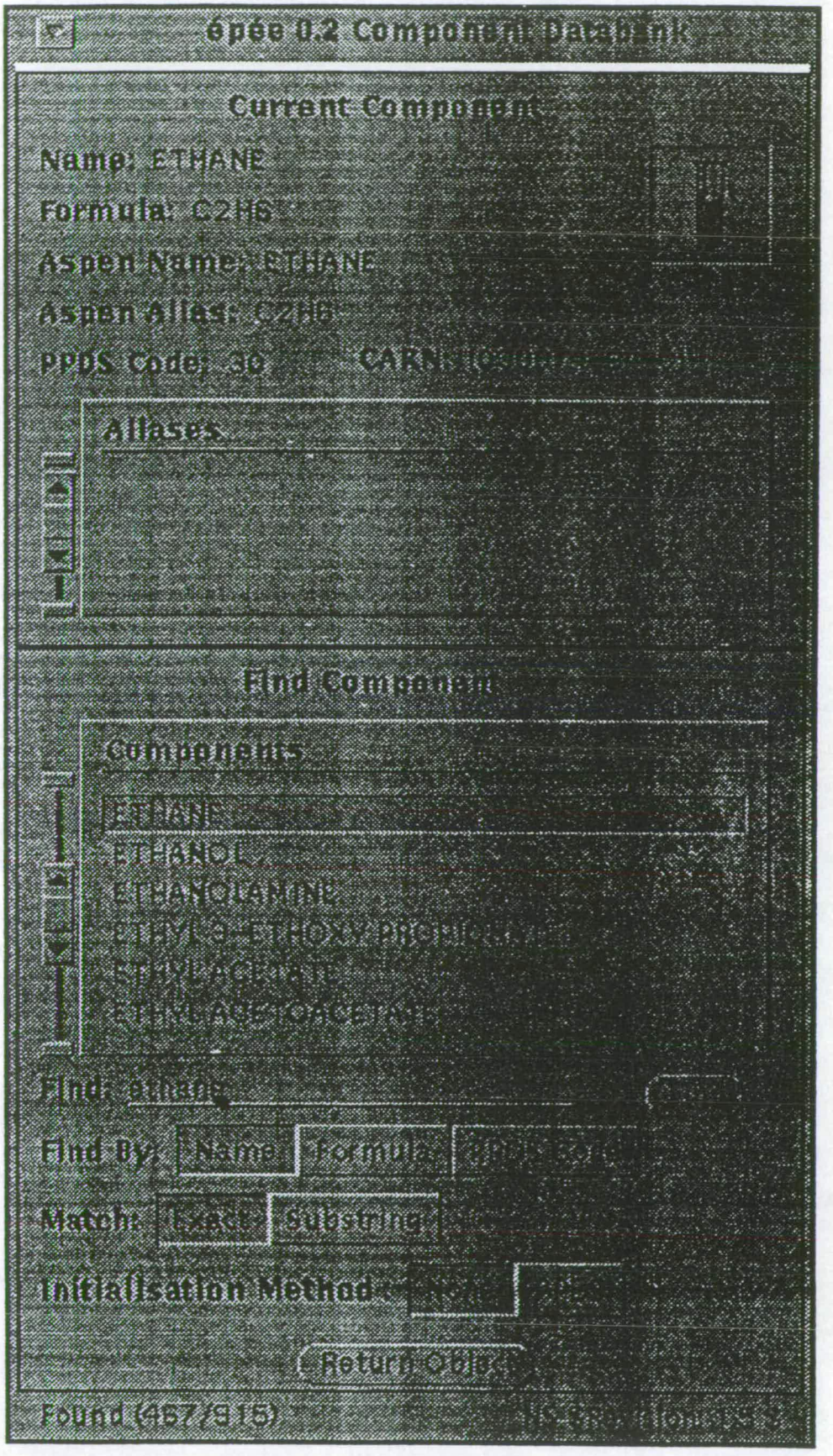

Epée 0.2 Slot Selector
Choose Slot
Unit_Type
Upper_Flammable_Limit
User_Unit
Users
Valence
Vapour_Entropy
Vapour_Heat_Of_Formation
Vapour_Pressure
varying_Parameter
Viscosity
VLE_Systems
VLE_Type
VLEquilibria_List
Volume
Y2ero_Inhibited
Type : Real
Dimensions : m 2 kg mol -1 s -2
Kind : MOLAR_ENTHALPY
Return Selection
Slot Selection Requested

Figure 18


Current Component
Name: ETHANE
Formula: C2H6
Aspen Name: ETHANE
Aspen Alias: C2H6
PPDS Code: 30
Aliases
Find Component
Components
ETHANE
ETHANOL
ETHANOLAMINE
Find: ethane
Find By: Name Formula
Match: Exact Substring
Initialisation Method
Return Objects
Found (467/915)

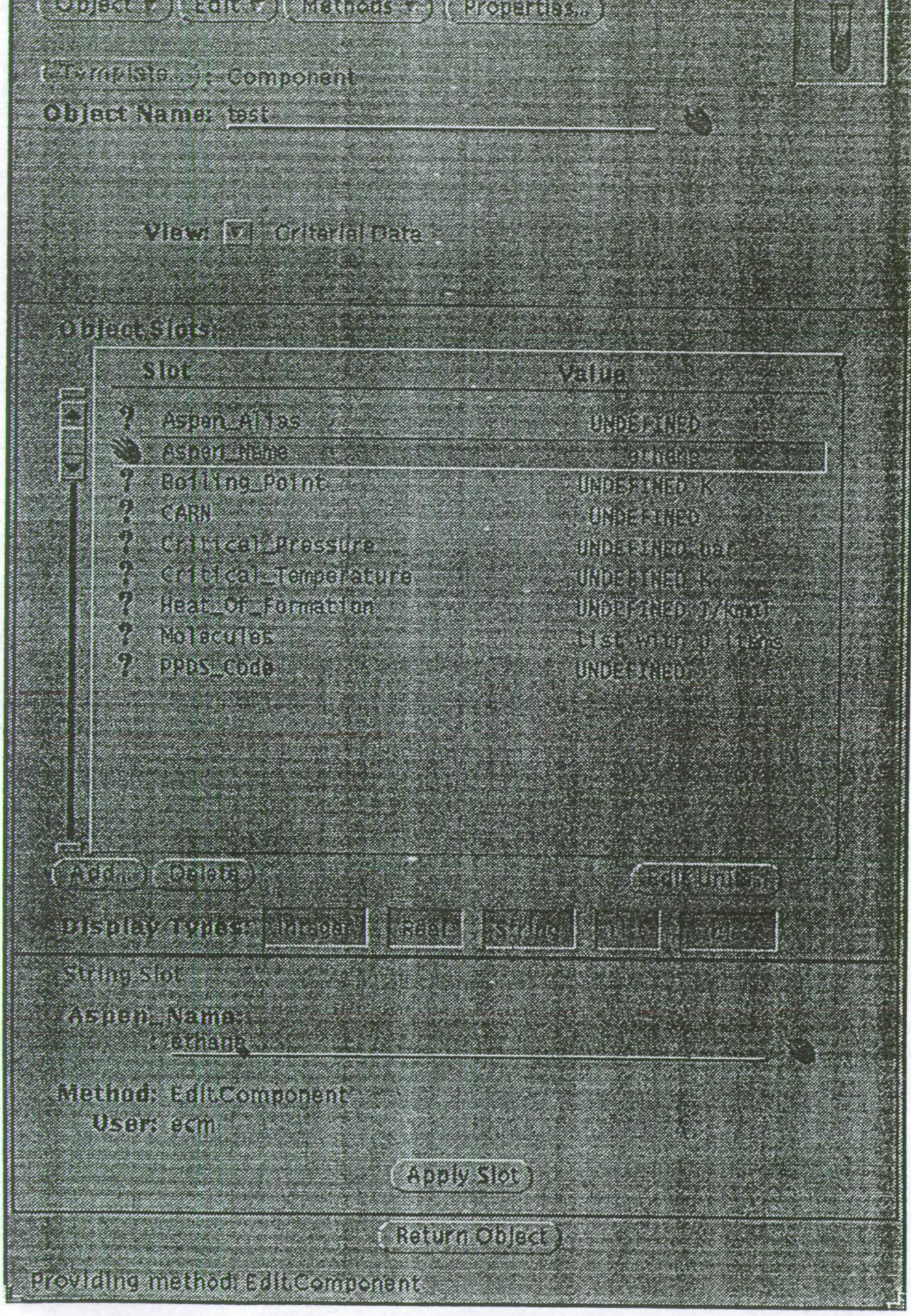
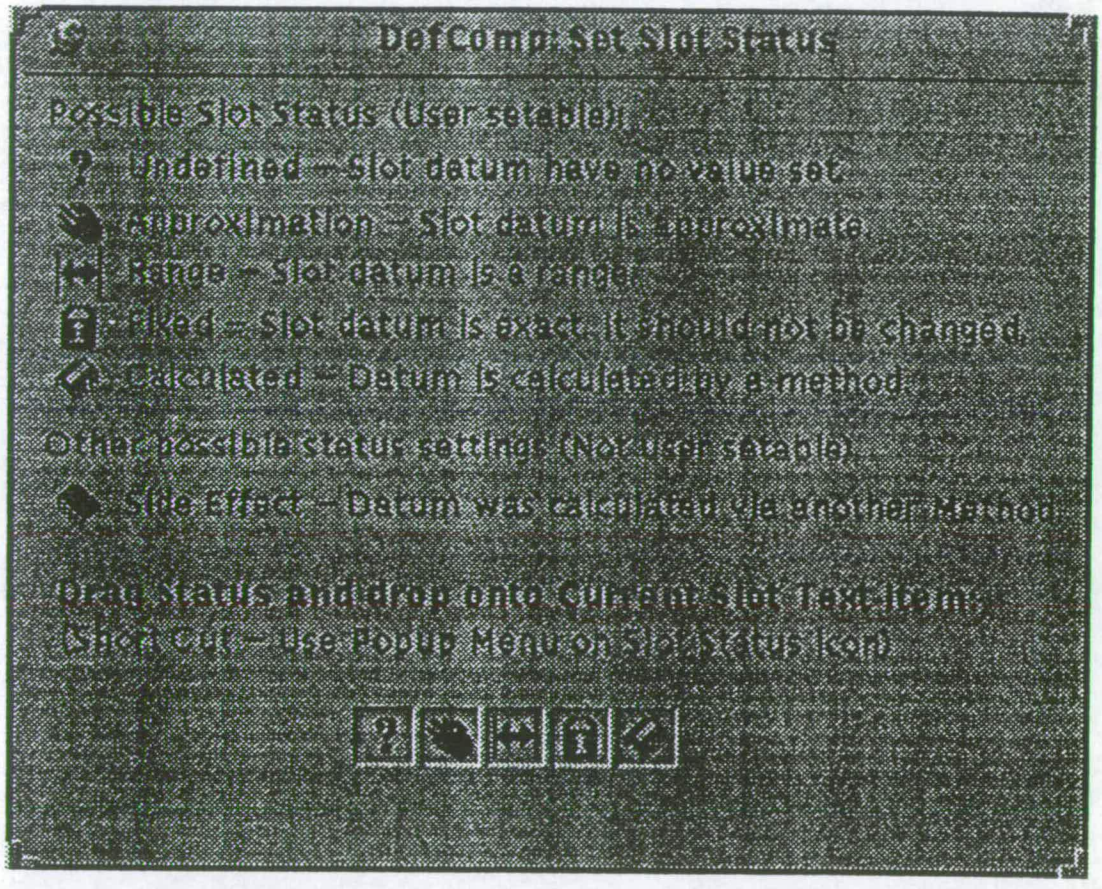

Object
Edit
Methods
Properties...
Template : Component
Object Name: test
View: Criterial Data
Object Slots:
Slot
Value
? Aspen_Alias UNDEFINED
Aspen_Name ethane
? Boiling_Point UNDEFINED K
? CARN UNDEFINED
? Critical_Pressure UNDEFINED bar
? Critical_Temperature UNDEFINED K
? Heat_Of_Formation UNDEFINED J/kmol
? Molecules List with 0 items
? PPDS_Code UNDEFINED
Add...
Delete
Edit Units...
Display Types:
Integer
Real
String
String Slot
Aspen_Name:
ethane
Method: Edit.Component
User: ecm
Apply Slot
Return Object
Providing method: Edit.Component

FIGURE 19

FIGURE 20


DefComp: Set Slot Status
Possible Slot Status (User setable):
? - Undefined -- Slot datum have no value set.
Approximation -- Slot datum is approximate.
Range -- Slot datum is a range.
Fixed -- Slot datum is exact. It should not be changed.
Calculated -- Datum is calculated using a method.
Other possible status settings (Not user setable):
Side Effect -- Datum was calculated via another Method.
Drag Stauts and drop onto Current Slot Text Item.
Short Cut -- Use Popup Menu on Slot Status Icon.

Chapter 8

Hierarchical Hazard and Operability Studies

8.1 Introduction

Every activity that humans undertake has an associated risk, be it staying at home in bed, driving to work or taking part in a rock climbing expedition. This risk is usually expressed as a fatal accident rate (FAR) quoted as the number of fatalities per 10^8 hours but it is also possible to express risk in other terms based on other consequences such as economic impact. Typical values, taken from (Kletz 1977), are given in Table 1. Advances in the handling of safety in many areas of life are resulting in a gradual decline in these figures. This trend can be clearly seen on the graph of ICI's fatal accident rate contained within (Kletz 1991). A number of serious accidents in the 1960's more than doubled the FAR for all risks from just over 3 to approaching 7. This highlighted safety performance and between 1968 and 1982 the all risks FAR fell steadily to just over 2. For process risks the corresponding figures are just over 1 in 1960 rising to about 4 in 1968 and falling to approximately 0.5 by 1982. If it is assumed that most humans do not have a death wish then they are continuously making decisions based on their assessment of the chances of the activities that they undertake causing them inconvenience or harm. Generally any negative aspects are balanced out against the need to undertake a particular activity and the positive aspects that will be derived e.g. whilst it is generally known that there is a greater chance of being killed whilst flying the wish to travel long distances in relatively short spaces of time is enough for most people to ignore the increased risk. The ability to exercise choice gives the illusion of being completely in control of the risks to which you are exposed but this cannot be the case due to the lack of control over the actions of others, acts of God etc. An important point to note is that the low FAR given for the chemical industry does not fit in with the general publics perception of the risk that it poses. To be cynical it would be better, from a public relations point of view, to allow a large number of small accidents killing only one or two people, as is the case with car accidents, and concentrate on reducing the major incidents which result in a large number of

fatalities. This push for an emphasis on high fatality accidents is highlighted by (Gibson 1977). However much such an approach appears to be infeasible, undesirable and unacceptable this is very loosely the reasoning behind hazard analysis which attempts to identify those elements of a project that pose the greatest threat in order to concentrate resources on addressing them. This simplification ignores the fact that there are many hazards that must be addressed but which would not, if they occurred, necessarily result in fatalities, here the use of an alternative consequence becomes necessary.

In a complex industry such as the chemical industry it is impossible to remove every risk due to the nature of the materials handled and the conditions to which they are subjected. However, many would argue that the aim should be to have a FAR of 0 and to this end it is necessary to identify, quantify and address risk issues during design. It has been argued, (Gadian 1974), that it is infeasible for the general public to expect such a performance from the chemical industry whilst readily accepting higher risks from activities such as driving and smoking on a voluntary basis, but this does not reflect the reality of the situation under which the industry operates. To deal with the apparent anomaly the principle of acceptable risk has been developed, (Gadian 1974 and Gibson 1977). Gibson suggests the adoption of a socially acceptable level of risk for processes and mentions a FAR of 2 for cases where all risks have been identified and 0.4 where there is remaining uncertainty. Quantification is the province of hazard analysis, which must follow on from hazard identification. Some people believe that "a hazard identified is a hazard controlled" (EFCE 1980) which implies that there is no need for quantification but this is a rather simplistic view that assumes that whose who have identified the hazard are fully aware of all the consequences. Even though hazard analysis will not be addressed in detail here this does not imply that the above view is believed to be correct. Lowe and Solomon support this view and state that although hazard identification is an important exercise if the knowledge necessary to handle the hazard is absent, or fails to be applied, then no benefit is gained, (Lowe and Solomon 1983). Kletz is of the opinion that HAZOP should be applied in all cases, but that HAZAN should be applied selectively, (Kletz 1992). He quotes a case where 326 HAZOP recommendations were raised but only seven justified HAZAN.

The identification of hazards and incorporation of means to address them into design will be discussed further in the remainder of this chapter.

8.2 Existing Study Methods

There has been a significant shift in attitudes towards addressing safety in design over the last thirty or so years. In 1960 the existence of a separate department concerned with safety was considered sufficiently unusual to merit a complete paper, (Thackara et al 1960). Today it is difficult to imagine a company that does not have staff, including those at a high level, dedicated to the formation and implementation of safety methodology and policy. The linchpin of current efforts to identify and address risk issues during design is the performance of a Hazard and Operability (HAZOP) study. Comparative methods, where a design is challenged by comparison with existing knowledge, have now largely been superseded. A HAZOP study is a systematic, critical, examination of a proposed process, on a line by line basis, developed by the Petrochemicals Division of ICI (Lawley 1974 and Gibson 1976) during the 1970's and subsequently generally adopted within the chemical industry. The driving force behind the development of the HAZOP methodology was a realisation that traditional, retrospective approaches were no longer satisfactory to address the scale of incident potential posed by modern plants. A comprehensive description of the technique is given in (CIA 1979) and (Kletz 1992). Although originally developed to handle continuous chemical processes the technique can be modified to handle batch plants, mechanical handling operations etc. A basic assumption of a HAZOP study is that the process will work well if operating under design conditions. The hazards arising from deviations from this state and the operability of the plant are reviewed. Design conditions and assumptions are not challenged in a systematic way but some will come under review in the course of a study. In addition to hazard identification benefits claimed for a HAZOP study are reductions in start-up modifications necessary and shortened commissioning times, (Roach and Lees 1981).

McKelvey identifies six key problem areas that can lead to difficulties when carrying out HAZOP studies, (McKelvey 1988). These are listed below in order of frequency of occurrence.

(i) Lack of experience within the team, with the role of the leader being key.

(ii) Failure to communicate, with incorrect P&IDs and poor operating procedures being highlighted.

(iii) Management failure to appreciate the time commitment necessary for subordinates.

(iv) Complacency. Frequently manifested in attitudes such as "It has not happened to us before so it is not worth considering".

(v) Shortage of the technical data, such as component physical properties, needed to make the necessary judgements.

(vi) Human failings due to lack of concentration etc.

These factors are discussed further below.

It has been pointed out, (Black and Ponton 1992, Ormond 1996), that a full line-by-line HAZOP study of a plant is demanding and difficult resulting in such studies being both time consuming and expensive. What is not heavily emphasised here, or in most of the texts discussing HAZOP studies, is that the real problem with them, that is that they are difficult to do well because they can easily become very boring, with most participants only being able to focus the attention needed for short periods of time. To obtain the optimum result it would therefore appear logical to carry out HAZOP studies in short bursts spread out over whatever time is necessary. Ormond suggests that good practice would be to limit meetings to a single half day session per day for a maximum of four days per week, (Ormond 1996). However due to limitations on availability of personnel, the costs inherent to assembling a frequently dispersed team and the need to meet project deadlines the time span needed for such an approach is likely to be an unobtainable luxury leading to long continuous study periods. Tightly packed review schedules run the risk of inducing boredom and frustration in a large team of expensive engineers which is counter productive and may lead to carelessness, oversights and possiblly cancels out some of the advantages of carrying out such an exercise.

The greatest benefit of the conventional way of carrying out HAZOP studies is that a team of people of different specialities and experience are placed together and focus on the plant in question, each approaching the problem from a particular

view point. The membership of a HAZOP study team varies as specialist disciplines are brought in to discuss specific processes or items of equipment but typically a core team would consist of a study leader, secretary, project process engineer, independent process engineer, project engineer, control engineer and a representative of the operator. Where equipment is being purchased as a package then one of the process engineering roles would be fulfilled by a vendors representative. It is now common for the secretary role to be fulfilled by the leader. Allowing meetings with a large number of attendees is expensive in terms of manhours and tends to cause long meetings if all participants are to be given an opportunity to contribute. Lowe and Solomon suggest a core team of four or five consisting of the leader, section design engineer, section process engineer, operating manager and instrument / control engineer. This team has to be supplemented as necessary by experts, (Lowe and Solomon 1983).

For a HAZOP study to be successful all team members must be familiar with the process and its purpose so that they can make effective contributions. Whilst the role of the study leader is pivotal the experience of other team members and access to experts is also critical. Significant operation experience and a good understanding of the nature of the hazards that are likely to be encountered have been highlighted as being particularly important, (Ormond 1996). The quality of the output, and hence safety of the plant, will be put in jeopardy if insufficient or inappropriate experience is available. In an exchange of views on the limitations of the HAZOP study technique, (Crawley 1995, Kletz 1995 and Tyler and Simmons 1995), this point was the main problem highlighted. Whilst a team cannot be expected to have a complete knowledge of all possible hazards the knowledge base should be sufficiently broad to allow creative thinking. Failures in HAZOP studies will arise, as there can be no guarantees with a technique that relies on abstract thinking, but these arise from the people applying the technique rather than from failings in the technique itself. In the authors experience the proposal made by Crawley that HAZID be incorporated into HAZOP already occurs. Suitably experienced teams will automatically question how a hazardous situation could arise. The result of such a gathering, ideally, is a great generation of ideas and proposed solutions, however to ensure that all the relevant points have been addressed and to avoid too much time

being wasted pursuing trivial details it is necessary to impose some form of structure on such a gathering. This imposition does run the risk of putting a break on the creative and exploratory aspects needed to ensure a high quality result is produced by the team. An unsystematic use of the method is likely to result in potential problems being missed. Highly structured hazard identification techniques such as check lists demonstrate the risks. Items outside the list are not considered and if any degree of innovation is present the results are likely to be incomplete. The traditional means of providing this structure is to undertake a systematic, line-by-line study of P&ID's which follows the steps outlined below, (Scott and Crawley 1992):

1. Select a line or system.
2. Define the design intention of the line.
3. Select a parameter to discuss.
4. Select a deviation that could occur in that parameter.
5. If the deviation is meaningful then find the consequences.
6. If the consequences could result in a hazard or an operability problem then investigate the possible causes.
7. If a realistic cause is found then assign an action to be taken.
8. Return to step 4 until all deviations have been examined.
9. Return to step 3 until all parameters have been examined.
10. Return to step 1 until all lines on the P&ID have been studied.

In addition to step 2 it is usual to have a project process engineer run through the purpose and design intent behind each P&ID before the HAZOP study on that drawing commences, for uncomplicated P&ID's this general description of intent is sufficient and step 2 need not take place for each line. This procedure focuses on the hazard identification aspect and does not make it clear how operability would be addressed. Such a situation is a common problem with HAZOP studies where the "HAZ" tends to dominate the "OP". The parameters and deviations used during a HAZOP vary between industry sectors, between companies within a sector and between projects undertaken by a given company. Using tailored lists of deviations can impair the effectiveness of a HAZOP study by limiting the area of search. As

pointed out by (Crawley 1995 and Tyler and Simmons 1995) the poor choice of guide words and parameters will seriously effect the quality of the study with the potential for hazards to be missed completely arising. Very careful consideration must be given to the selection of an appropriate set of parameters. Table 2 gives a typical list of these factors and gives a brief outline of the meaning of the deviations. Whilst using slightly different deviations, also termed guide words, (Coulson et al 1983) gives a good background discussion of the HAZOP study technique. It should be noted that not all possible combinations of parameter and deviation can be considered to be feasible, e.g. applying "part of" to temperature or pressure, and that a well run HAZOP meeting with an experienced study leader will intelligently apply the steps outlined above rather than simply slavishly following them. Such an approach can reduce the time spent on a study, help to keep the attention of the team members and ensure that the study members do not fall into the trap of thinking that simply identifying all the possible hazards without regard for their feasibility is sufficient. Never the less performing a line by line study is a lengthy and repetitive task during which it is difficult to maintain a sufficiently high level of motivation and participation from team members. This can be exacerbated by the fact that although the study is carried out on a line by line basis no line is a completely separate entity leading to the need to carry forward the consequences arising from the line under study forward and backward to other lines so breaking the continuity of the study.

Shifts away from full attention being paid by team members could result in potential problems being missed or glossed over, however, to the degree of redundancy built into the technique and the number of participants makes it unlikely that an unsafe system would result. The redundancy arises from the fact that a hazard may be identified from the application of the guide words to more than one line and, as pointed out by (Rushton 1989) represents a weakness as well as a strength of HAZOP studies. It is a weakness because it can lead to a feeling of frustration amongst the participant arising from the fact they appear to be asked to reinvestigate hazards that have been dealt with previously rather than making progress. This leads to a feeling of repetition which can be minimised by a study leader who keeps control of the meeting and rapidly halts re-examination of issues and stops discussions wandering off at a tangent. An analysis of time usage in

HAZOP studies carried out by Jefferson and co workers noted wide variations in the time spent discussing, in particular, the actions that should be taken and equated this to the control which the leader exerted over the meeting, (Jefferson et al 1995a).

Whilst such a systematic approach is comprehensive it would place an enormous burden on those involved in a HAZOP study if no attempt to address hazard and operability issues were made until firm P&ID's had been produced. An additional draw back of this approach would be the check imposed on project progress by the need to delay the study until such drawings and the necessary supporting documents became available. Such a delay is inherent in the design process as firm information can only be produced when the bulk of the design work has been completed and all holds have been resolved. The supporting documentation that must be available to back-up the information contained on the P&IDs is listed below and gives a good indication of the level of design work that must have been undertaken before a traditional HAZOP study can be carried out.

1. Preliminary operating instructions covering all modes of operation, start-up, normal, shut-down and upset. These are necessary to determine intent and act as a basis for identifying the likely reaction to upset conditions.
2. Preliminary maintenance instructions. These are used to ensure that the facilities, such as drain down lines and sufficient access, are available to allow maintenance to be carried out safely.
3. Equipment specification sheets giving details of the function of plant items and the design parameters. These are used to address performance and limit questions that may arise during the study.
4. Instrument list with details of normal settings. Necessary to define the expected values of the operating parameters.
5. Trip and alarm system description including settings and sequences. This information is needed to determine the reaction of the plant to disturbances and upset conditions.
6. Control system architecture. This is used as a reference document during the study to aid understanding of the intended control regime.

The preparation of this documentation requires the efforts of a multi-

disciplined team, with heavy control and instrumentation input, over a considerable period of time. Failure to have all the necessary documentation available could compromise the quality of the study, (Tyler and Simmons 1995), but in the push to complete the studies and freeze design such considerations run the risk of being sidelined. Care must be taken to avoid reducing the exercise to one of simply ticking the box that says reviews are complete. As operating details only become available when the design has progressed to a certain extent, particular care has to be taken to ensure sufficient information is available to allow operability to be addressed satisfactorily.

Consider the manhour effort and cost involved in undertaking a traditional HAZOP study. Each P&ID can contain a large number of lines, not untypically 50 and in exceptional circumstances up to 100, and each project has a large number of P&ID's, up to 90 for a relatively complex single stream plant with associated utilities and off-plots. For a core team of 7, defined above, spending 15 minutes per line on a medium size job containing 50 P&ID's with an average of 30 lines per drawing the total manhour expenditure would amount to 2,675 hours. Given a manhour rate of £30.00 per participant the cost of such an exercise would be £80,250 excluding overheads, travel etc. The time involved per P&ID, 7.5 hours, leads to a total of 375 hours or 9.375 working weeks per participant, based on a 40 hour week. Given that the number of drawings and lines for a project are fixed then the only remaining variables available for the reduction of cost and hours are the number of team members and the time spent per line. In order to maintain the quality of the output it is undesirable to reduce the number of team members, though perhaps one of the process engineers could be removed, therefore the only remaining factor is the time spent per line. For each minute reduction in this duration the savings in the above example are £5,250 and 25 hours per participant. Freeman and co workers describe an expert system developed by Monsanto for estimating the time required to carry out HAZOP studies, (Freeman et al 1992). Based on the number and complexity of flowsheets, number of people in the meeting and skill of the leader the total time, including preparation and report writing, can be determined. This allows planning of the required effort and time scale, based on three to four meetings of up to 6 hours per week. For an average leader an average time scale of 6 hours per P&ID

is estimated. Given the relatively simple task involved it is doubtful if such a system would add sufficient knowledge to be of significant help. Jefferson and co workers analyzed the pattern of time usage in 11 hazard studies to determine if the process could be speeded up without affecting the quality, (Jefferson el al 1995a). They did not identify any opportunities for such reductions but noted that the level of experience of the leader coupled with the control exerted over the meeting both impacted on the time spent. These findings are not surprising. To achieve a substantial reduction in time spent whilst ensuring that the quality of the design product is not compromised requires a re-examination of way in which hazard identification is addressed during design. Care must be taken to ensure that the drive to reduce costs does not dominate and belittle the need for a safe design product.

It has been recognised since the use of HAZOP studies were still relatively new (EFCE 1980) that much of the literature about this technique implies that this is the only hazard identification study undertaken. Due to the number of times that this idea has been implied there is a tendency for it to be adopted as correct by some. The confusion arises due to the fact that in addition to studies that are specifically referred to as HAZOP a number of other reviews that impact on the same concerns take place during the design process. These reviews, such as Trip and Alarm reviews and P&ID reviews, tend to be focused on a rather narrow range of concerns but all have a contribution to make towards overall safe plant operation. The most common current position is that whilst a traditional, line by line, HAZOP study is not the first, or only, attempt to identify hazards it forms the mainstay of such procedures. As hazard identification at the P&ID stage represents an ideal opportunity to check that hazard control has been applied correctly during design and development and to provide a foundation for operating procedures this situation is not entirely undesirable. The majority of those involved in hazard identification for projects consider HAZOP studies to be the best technique available, (Turner 1996), but feel that there is room for improvement. Turner reports on a workshop held by the Safety and Loss Prevention Subject Group of the IChemE which resulted in five major conclusions about the current state of the technique:

1. An industry HAZOP study standard should be agreed covering all aspects of the study including team composition, training, documentation used,

recording and action implementation.

2. All HAZOP studies should be audited against the agreed standard to ensure compliance and demonstrate effectiveness.

3. The use of computerised recording of HAZOP studies and the actions arising should be considered for all studies. The benefits claimed include an inherent audit trail, increased speed of production of agreed study notes and ease of chasing follow-up actions.

4. A lessons learned database containing information about previous incidents has the potential to make up for lack of knowledge or experience within the review team by providing on-line searches for similar situations during hazard identification.

5. Three quarters of the delegates at the workshop considered that HAZOP studies are a cost-effective technique.

There is a tendency to view the HAZOP review procedure as a hurdle that has to be overcome rather than an aid to the design process. This primarily results from the use of stages that do not concentrate sufficiently on the early phases of design, causing safety to be an expensive add-on rather than an inherent feature. If a large number of actions are raised by a classic HAZOP study this should be viewed as a failing in design procedures and not accepted as a means of "catching" issues. Additionally further burdening design team members at one of the busiest phases of a project will not guarantee a high quality of responses to actions. The temptation to consider a problem as solved by simply assigning an action should be resisted and the need for adequate follow-up cannot be emphasised strongly enough.

Not withstanding the acknowledged advantages of the HAZOP study technique the costs and time involved have resulted in the proposal of a number of approaches aimed at reducing the burden imposed. These can be split into three main groups hinging upon either performing the required study in a hierarchy of stages taking place over the life time of a project, providing support for the process or upon automation of the procedure. Each will be discussed in turn below.

Reviews involving multi-discipline teams are not the only forms of hazard identification that take place over the life of a project with other available techniques,

(Lowe and Solomon 1983, Jones 1992), being fault tree analysis, event tree analysis, failure modes and effect analysis, cause-consequence analysis and various indexes. These are generally carried out by individuals with the aim of providing quantitative data to be used as a basis for other work. Jacobs identifies four techniques, What-if Checklists, Failure Mode and Effect Analysis, HAZOP and Fault Trees, used by Du Pont for process hazard reviews, (Jacobs 1989). Of the four HAZOP was the newest technique being used at the time and Jacobs implies that it was not routinely applied to all jobs. The review procedure adopted by Du Pont was to assemble a review team consisting of operations, maintenance and technical personnel and apply one or more of the review methods. It has been noted, (Dimitriadis et al 1995), that the lack of quantitative content within the HAZOP technique can lead to efforts being expended on relatively minor problems at the expense of those that have the potential to be much more serious. This view point fails to acknowledge the interaction between the existing quantitative techniques and the HAZOP study process. The most commonly occurring indexes, the Dow Index (Dow 1981) and the Mond Index (Lewis 1979, Doran and Greig 1989), were developed to allow the potential hazards of a process to be evaluated and the necessary safety and loss prevention measures to be assessed at an early stage in the design process. The Mond Index is a development of the Dow Index which aims to cover a wider range of units including the evaluation of a toxicity hazards index in addition to fire and explosion indexes, (Tyler 1985). The emphasis on toxicity has subsequently been reduced. Fault tree analysis is the most generally used of the three analysis techniques mentioned and works from a top event back through a number of layers of contributory events, via a system of gated branches, to all the possible initiating events. A separate tree is required for each top event considered and is first synthesised by study of the plant in question before being analyzed. This analysis can be simple qualitative but routinely the frequencies and probabilities of the contributory events are used to determine the frequency of the top event. Fault tree analysis adopts a top-down approach towards hazard identification and it has been pointed out, (Black and Ponton 1992), that prior to HAZOP studies, which are bottom-up, all hazard identification is on this basis. The scheme for reviews prior to HAZOP study proposed by Wells and co workers, (Wells et al 1994), does not move away from

this and claims as a benefit the ease of preparation of fault trees. Only more general qualitative techniques, such as HAZOP, will be considered further here but it should be noted that in addition to the commonly used tools for the qualitative analysis of fault trees attempts, have been made to automate the synthesis of the trees. Early work by Kelly and Lees resulted in the FAULTFINDER code, (Kelly and Lees 1986 a, b, c and d), which used fault propagation models of the plant elements as the basis of the synthesis. Parmar and Lees also consider the propagation of faults through a plant but concentrate on hazard identification, (Parmar and Lees 1987 a and b). The integration of this type of work and code into a CAD environment is discussed by Khan and Hunt, (Khan and Hunt 1989). Waters and Ponton also discuss the computerised simulation of fault trees, (Waters and Ponton 1989). For most designs the production of fault trees for the whole plant would not be attempted but work would be focused on areas of particular concern. HAZOP studies do include some degree of fault path detection but the exploration is unsystematic and fragmented. Whilst work has been done to attempt to produce fault trees from HAZOP study notes of meeting, (Roach and Lees 1981), the incomplete nature of the exploration means this is unlikely to be successful.

8.3 Staged Study Procedures

Rather than relying on a single pass to pick up all the relevant points adopting a staged approach allows a number of, hopefully, shorter studies to take place. Even before the HAZOP study procedure had been proposed the need for a staged approach towards design safety had been identified, (Thackara et al 1960), and this was further enforced during the early days of the development of the HAZOP technique as noted by (Gibson 1976), (EFCE 1980) and (Lowe and Solomon 1983). The latter recommended that project approval procedures should include the requirement for potential hazard reviews at appropriate stages from the inception of the project, through project completion and during the life of the operating plant. As should be expected initial attempts to put this into practise generally fell some way short of target and commonly relied upon a two stage procedure, although (McCrindle 1977) does briefly outline five stages. In addition to the P&ID HAZOP study a "coarse" HAZOP study was carried out at the PFD stage, as mentioned by

(Scott and Crawley 1992), using a modification of the basic technique. This modification is applied to each PFD as a whole rather than on a line by line basis and has additional parameters and deviations based around unit operations. Such an approach is no advance over that described by (Thackara et al 1960) which although referring to safety studies rather than HAZOPs does include the use of check lists for hazard identification. One early attempt to focus on hazard identification in the conceptual design stage is described by (Pyman and Mitchell 1982). They identify three criteria that any method to identify hazards during the conceptual phase of design must fulfil, these are that it must be systematic, to allow confidence that all areas have been covered, that it must identify hazards from all sources and that it must concentrate on major areas of concern without being side tracked into irrelevant detail. The procedure proposed comprises of four stages running from the subdivision of the plant, specifically an off-shore platform, into areas, through the use of check lists to identify potential hazards and the use of a coarse HAZOP study to a qualitative review. The coarse HAZOP study is carried out by a much smaller team than for a full HAZOP study, due to the lack of information available, and it is claimed that the study produces useful guidelines for the later design and significant feedback into the design process. Unfortunately no case study material is discussed.

Ideally whatever the approach adopted to hazard identification the resultant design should have the same level of safety but using a staged method is expected to result in improved levels. This arises due to both the greater number of opportunities for factors to be identified and the increased chances of design changes taking place to address these factors. The earlier in a design that hazard identification studies start then the more fundamental the changes that can be made to the design to address points raised without incurring a heavy time delay or cost penalty. This need was acknowledged before the HAZOP technique had been developed. Claydon concentrates on the economic penalty of installing unsafe as opposed to safe plant but emphasises that it is necessary to appraise processes from the earliest stages of their development to ensure a balance between these two factors, (Claydon 1967). Although specifically discussing food hygiene (Hastings 1995) emphasises this point by stating that consideration of the relevant factors from the onset of a project will

enable many potential problems to be eliminated at the design stage with minimal cost. There are however disadvantages of carrying out a study at an early stage in the design process when the design is not fully developed. The relative merits of timing HAZOP studies at late and early stages in design are considered by (Turney 1990) whilst discussing the development of the six stage hazard study procedure used by ICI. Carrying out a full HAZOP study at an early stage presents the maximum opportunity to consider an inherently safe design but due to the lack of thought out design detail there is a danger that the study meetings become design meetings resulting in a sufficient level of change to require an additional study to examine the final design. This represents a move towards a two staged approach. As discussed above, Turney points out that a single HAZOP study carried out late in the design means that the design is highly inflexible leading to safety only being achieved by bolt-on systems rather than being inherent. There are however benefits in this approach as the study is carried out on a largely defined design and thus acts as a check on the design process. A staged approach using modified studies allows the benefits of both approaches to be obtained whilst avoiding the drawbacks.

Currently used approaches, such as that described by (Gillett 1995), have moved further towards the goals originally identified and consist of a number of stages, but they have a tendency to start too far into the design and to contain only a few steps to cover the project from feasibility studies through to detailed design, the design phases. Whilst studies carried out late in detailed design and during the commissioning and operating phases may be useful for learning lessons about the problems that have occurred during the design they are more likely to benefit later projects, if lessons are learnt, than the project for which they are carried out. The same accusation could also be levelled against the five stage procedure discussed in (McCrindle 1977) where three of the stages occur during, or after, detailed design. Gillett describes a six stage procedure for undertaking hazard studies, the stages used are described in Table 3, where four of the stages occur after the bulk of the design work has been completed and three after design is complete. The same procedure is discussed by Turney who names it as that developed by ICI during the mid 1970's, (Turney 1990), and by Ormond who claims that the effectiveness of HAZOP is greatly enhanced by the preceding studies, (Ormond 1996). Hazard study 2 as

described by Gillett occurs before the P&ID's have been produced and is based on the application of deviations to a block flow diagram of the process. This corresponds to the first stage of the two stage procedures discussed above with hazard study 3 being a traditional HAZOP study. Turney emphasises that the study procedure developed by ICI allows a combined approach to safety, health and environmental protection, hence the common acronym SHE. This is in line with the developing legislative burden and represents the best way forward.

Lihou claims that for smaller companies and projects a six stage procedure can be excessive, (Lihou 1990), although it should be noted that such applications have been reported. He proposes an alternative three stage procedure based on Conceptual, P&ID and Task HAZOP studies. The Conceptual HAZOP study focuses on each major equipment item on a PFD and undertakes what is termed a "Process Deviation Analysis" by asking high level questions on intent and causes of failure. The P&ID HAZOP study is close to a traditional review with the addition of severity indexing to rank hazards. Lihou emphasises the need for good description of intended equipment and control system performance at this stage. The final stage proposed by Lihou, Task HAZOP study, covers operability and maintenance aspects. These are elements that should be covered in a full HAZOP study of the P&ID and it is doubtful if it is desirable to separate the two elements as they are strongly interrelated.

Delaying the start of hazard identification may preclude the making of fundamental changes that would eliminate hazards entirely or the cost of implementing changes becomes prohibitive. Failure to eliminate hazards makes it impossible to achieve inherent safety in a design and places a reliance on engineered solutions to limit the hazards. Whilst this in itself should not result in plants where safety is compromised the additional equipment and instrument items add to both cost and complexity. There are however a number of accidents that can directly be attributed to failings of designed in safety systems. Most notably both Seveso and Bhopal resulted from the functioning of pressure relief systems that protected the plants but caused releases of toxins into the atmosphere. Such incidents have led to an interest in designing plants without pressure relief streams. Wilday gives a run down of the methods that can be used to move towards this goal, (Wilday 1991), but

states that such plants are currently not possible. Areas of difficulty are external fire protection, atmospheric storage tanks and certain chemical reactions. In a survey of literature and interviews to establish company attitudes to addressing safety in design, (Mansfield and Cassidy 1994), the impression gained was that safety is often only addressed late in the design, at a HAZOP study on P&IDs. Any earlier studies uncovered tended to focus on hazard identification and control rather than the elimination or reduction of the hazard. Such an approach fails to embrace the concept of inherent safety.

Wells and co workers at Sheffield propose a series of reviews aimed at improving the safety reviews carried out prior to HAZOP studies, (Wells et al 1994). Their work hinges on the identification of causes that could result in a release of process material to the environment. The first review proposed by Wells et al is a Concept Hazard Analysis which uses a series of guide words to primarily consider the consequences of a material release. This is very similar to the first stage of the ICI procedure. In addition to material based hazards a Process Sociotechnical System Analysis is proposed to consider the resources needed for the project and the interaction between the project and the environment in which it will take place. When preliminary P&IDs are available Preliminary Hazard Analysis takes place. Here a release to atmosphere is taken as the top event in the analysis and a top-down approach is used to identify the causes. This is a similar approach to that used in developing fault trees and this is claimed as a benefit of the technique. A co-incidental Preliminary Consequence Analysis examines the impact of a release and produces an event tree. Following the completion of the Preliminary Hazard Analysis a Process Safety Sociotechnical System Analysis is proposed. This emphasises the individual, social, organisational and managerial facets of the plant and the impact that they will have on the safety performance. The overall system is split into subsystems covering areas such as management control, procedures and practices, site and plant facilities and operator performance. To each of these subsystems keywords are applied to highlight possible safety issues. The analysis, as shown by an example is, by virtue of the relatively low level of information available at this stage in the design, rather superficial. The emphasis is exclusively on major safety issues with releases to atmosphere dominating. If expanded to cover

other SHE concerns the review schedule proposed would provide a comprehensive approach to be used during the initial stages of design. Essentially four stages are proposed prior to HAZOP studies.

The basic concept behind the inherent safety principles first proposed by (Kletz 1984) is to avoid hazards rather than control them which, at a very simple level, can be encapsulated in phases such as "What you don't have, can't leak", "What you don't have cannot hurt you" etc. At this level the concept of inherent safety was acknowledged long before, (Matheson 1960 and Gadian 1974), the work by Kletz defined the five categories, given below, which can be used to ensure inherent safety is considered during design. The early phases are particularly important as fundamental changes can still be made. Kletz proposes the use of check lists to ensure that inherent safety is considered. Given the length of history of the approach the slow pace of take-up is disappointing. Kletz also claims that inherently safe plants are cheaper because of the reduction in add-on safety equipment and the diminished physical scale. For added-on equipment maintenance costs have to be considered in addition to the capital cost. To have a significant impact on the design all five must be examined during the early stages. Edwards and Lawrence discuss the application of a technique to rank route alternatives in terms of inherent safety and compare the results with the rankings given by human experts, (Edwards and Lawrence 1995). To keep abreast of legislative changes it is also necessary to consider ways of designing plants that possess inherent environment friendliness and inherent hygiene. Mansfield and Cassidy point out that an inherently safer process may not be more environmentally friendly if the life cycle of a product is considered, (Mansfield and Cassidy 1994). Care must be taken to avoid imposing conflicting demands on a design.

1. Attenuation: If a hazardous material cannot be avoided use it under conditions that reduce the hazard. eg dilution with an inert material, reduce the temperature or use a lower pressure.
2. Intensification: Reduce the inventory of hazardous materials to the lowest possible level.
3. Limitation of effects: Design safety into the main design and avoid the use of additions to the design to address it.

4. Simplification: Avoid making the design overly complicated as this will increase the likelihood of misunderstandings and mistakes leading to hazardous situations.

5. Substitution: Whenever possible avoid the use of a hazardous material and use one that presents a reduced hazard.

A number of examples where inherent safety was achieved by careful consideration of the manufacturing route are given by (Kletz 1984) and (Rogers and Hallam 1991). These are based on substitution, the most satisfactory way of achieving inherent safety. Snyder discusses the application of inherent safety within the USA, (Snyder 1996). He considers that the role of operating personnel from the earliest stages of design is a key factor in achieving an inherently safe plant. Simply sticking to an ever growing list of international, national and corporate standards will not result in such a design and may cause confusion amongst those asked to follow all the paperwork. Snyder also emphasises the criticality of staged hazard study procedures.

To increase awareness and application of inherent safety principles in industry the HSE commenced a sponsored project in 1992. Mansfield and Cassidy report on the first two of the three phases of the initial pilot study but do not cover the application of the tools developed to industrial processes, (Mansfield and Cassidy 1994). The initial survey phase highlighted a general lack of awareness of inherent safety issues and identified the need to develop practical measures to help companies address these issues during design. To this end a framework was developed to challenge the basis of a project in a systematic way from the earliest stages. This framework is discussed in Chapter 4. Using this as a basis the project concentrated on developing tools to address safety in the early stages of design. The stages used do not link directly to the project phases outlined in Chapter 1. Initial specification and Process Synthesis Route would occur during Feasibility Studies. Chemical Flowsheet and Process Flowsheet constitute Conceptual Design and Process Conceptual Design corresponds to Front End Design. Tools to address inherent design during these first four stages of the framework are described by Mansfield and Cassidy along with a ranking index to aid the selection of the alternatives. No case

study work is described. At the first stage the tool proposed is a structured brainstorming technique to challenge the need for the product and the means of fulfilling that need. A screening process based on safety, practicality and economic and technical feasibility is used to select and rank the most promising options. The synthesis route is challenged using a prompt checklist during the second stage. Issues covered include items such as the use of different pressures or temperatures, use of an alternative solvent or catalyst or the use of natural versus recycled versus synthetic materials. Screening is based on the hazardous properties of the materials involved and the reactions between them. The chemical flowsheet is then challenged using a modified form of the HAZOP study technique. The guide words used are split into two groups which challenge the materials and the conditions respectively. Any alternatives generated are given a score of +, 0 or - relative to the original scheme to provide a screening process. A modified HAZOP study technique is also proposed for the fourth stage considered. The process is broken down into building blocks, each with a defined function. Guide words are applied to determine if there are alternative ways of achieving the same function. A second set of guide words applied to the blocks examines if changes in timing, sequence and physical or chemical conditions can improve the process. Alternatives are evaluated in terms of their safety benefits and feasibility. The proposals represent a raft of techniques which appear to have the potential to improve the design quality. However, the lack of any case study information makes the impact difficult to judge. Tyler proposes the use of the Mond Index for ranking the inherent safety of alternative routes and includes an example, (Tyler 1985). This would seem to be a simple approach but the qualitative nature of the various rankings within Mond may make it difficult to compare alternatives.

Another major project in this area is STOPHAZ under the EC ESPRIT III programme. The STOPHAZ project started in December 1993 with the aim of developing a set of support tools for use in safety related design and operation, (Preston 1995). It was also intended to investigate how such tools might impact on hazard study methodology and the unification of the various alternatives. Ten partners from seven European countries are involved with ICI as the project manager. The first task undertaken was to conduct an industry wide survey of user views and

needs to establish a firm foundation for the tools to be developed. Preston gives a summary of the results of the survey and the conclusions drawn, (Preston 1995). The dominant issues and problem areas identified were:

(i) Poor integration and communication between various departments leading to repetition of safety problems.

(ii) Poor corporate memory leading to problems in learning from safety incidents.

(iii) Lack of inherent SHE in design, pinpointed as being the result of the late involvement of SHE practitioners in design. This could be viewed as spurious as it divorces safety from the main stream of design.

(iv) Lack of adequate operating instructions at HAZOP study.

(v) Personnel deficiencies, competence and availability, during HAZOP study.

(vi) Problems with studying programmable electronic systems (PESs).

Detailed analysis of the survey results identified three key areas where computer tools could provide the greatest benefit to those undertaking safety related design. Preston and Richards give a report on the functional modules proposes within STOPHAZ to address these areas, (Preston and Richards 1995). These are discussed in turn below:

(i) ELDER (ELD helpER). ELDER aims to offer the developer, or checker, of an ELD (P&ID) advice to assist them in determining the suitability of process equipment configurations to meet SHE criteria. As well as access to legal codes and standards the framework to allow incorporation of corporate rulings will exist.

(ii) HAZID (automatic HAZard IDentification). HAZID is an automatic hazard identification module aimed at the identification and reporting of feasible and important hazards inherent in the design of a chemical process plant. The approach style emulates HAZOP studies, with similar data requirements, and whilst time advantages are anticipated the elimination of a conventional study is not a primary goal. Visible output is planned to be tables similar to those produced by HAZOP studies and an invisible database

of cause-to- consequence chains.

(iii) CHOPIN (Computerised Helper for OPerating INstructions). CHOPIN aims to assist in the development of effective operating instructions.

To maximise the potential user base STOPHAZ will be targeted at a Windows PC platform. The architecture employed is of a user interface providing access to the three modules mentioned above, databases, a plant description tool and CAD. Trials on the first prototype of STOPHAZ were planned for Summer 1995 with a second prototype following a year later. Initially only ELDER and HAZID will be implemented.

Even after taking the above into consideration there will always be situations where the use of hazardous substances or conditions cannot be avoided. In such cases design safety measures must be applied to mitigate the hazardous properties.

The increased cost of making changes as the project progresses is emphasised by (Kletz 1988) who focuses on the need to make plants more able to tolerate departures from normal conditions without moving into a region of operation that is either unsafe, unstable or inefficient. Plants with such a characteristic are said to be user friendly. The following breakdown of cost implications is given:

"For every £1 it costs to fix a problem at the conceptual stage it will cost:

	£10	at the flowsheet stage
	£100	at the detailed design stage
	£1,000	after the plant is built and
over	£10,000	to clean up the mess after an accident."

The impact on schedule and cost of taking decisions at the various stages of a project is also discussed by Nelson and co-workers when describing a team based approach to the management of large refinery projects called Cooperative Design Process, CDP. CDP aims to address the difficulties inherent in the coordination of such large scale activities and claims are made that both the efficiency of execution and probability of achieving a profitable plant are improved, (Nelson et al. 1995). A key advantage claimed is that having a team made up of the various interested

parties, owner, licensor and contractor, involved at all stages allows good quality decisions to be made with the minimum of delay as all the required expertise is readily available. If these "good" decisions are taken early then the cost of the change is low whilst the ability of the decision to impact on the successful project outcome is high. As a project progresses the impact of the two factors shifts and by the time that the plant is in operation the cost of change is high whilst the impact is low. The early identification of potential hazards allowing the principles of inherent safety to be applied and environmentally sound equipment to be selected is specifically highlighted as having a major impact on the possibility of achieving a profitable plant.

One common terminology used by staged approaches is that all stages are referred to as hazard studies. Whilst this is generally meant to refer to other hazards as well as safety the term is open to incorrect interpretation and may lead to an important function of the original HAZOP technique, that is to say the addressing of operability and maintenance issues, being sidelined. This danger has been identified and the importance of obtaining the experiences of people who have operated and maintained similar plants emphasised, (Turney 1990).

It should be noted that there is an inherent danger of "review fatigue" with a staged HAZOP study approach as many other studies, such as P&ID reviews and instrumentation reviews, are also required during design. Many of these reviews are related to a traditional HAZOP study and they ensure that documentation needed to carry this out are in order. As such they should be an integral part of the staged HAZOP study approach with clear progression and lines of responsibility. There are several points where care is needed when setting up a staged procedure. Firstly it is essential to avoid imposing such a high burden of reviews that there is no time to actually do the design. Secondly the review structure should be sufficiently flexible to avoid a "tick the box" attitude where it is seen to be essential that all reviews are carried out in a rigid order and time frame even if they are not applicable to the job in hand or the state of the design at a given stage. In both these cases there is a very real danger that the review process is devalued and reduced to the level of a sideline activity, that is undertaken because procedures say it must be, rather than an integral part of the design process. Such a situation negates the impact that the HAZOP

reviews should have on the design product.

8.4 HAZOP support tools

As plants have become more complex, in terms of the processes involved and the control schemes applied, it has become increasingly difficult for HAZOP study teams to follow the impact of a guideword through the system. A variety of approaches aimed at reducing the burden have been proposed. Tools provided to support the HAZOP study process can be split into three classes; those to aid recording of meetings, discussions and actions, those to provide support for the meeting process and those to provide expert assistance to the review team. These are discussed in turn below.

8.4.1 Recording of meetings, discussions and actions

Traditionally the recording of HAZOP studies was done manually by a junior member of the design team with one of two approaches being adopted to the level of detail entered into the formal records. For the most complete record a summary of all the parameter and deviation combinations considered is noted even when no consequences or causes are identified. This results in long and rather tedious notes but an auditable trail is left to prove that procedures were carried out correctly. Alternatively recording only takes place when a consequence and cause are identified and an action assigned. This results in much more concise notes but large gaps in the audit trail. Whilst the quality of the HAZOP study is not related to the completeness of the record, such an account does allow some form of quality assurance to take place. Additionally it is helpful when a HAZOP study has to be reworked for a modification. Whilst discussing the application of Total Quality Management to Hazard Studies and their recording Turney gives a guarded endorsement to the use of computer recording systems, (Turney 1991). To eliminate the need for handwritten notes that then need to be typed up for issue there are a number of packages available, such as HAZSEC (DNV Technica 1995), that allow direct typing into customised forms that can then be printed out immediately to act as the study report. Making use of computers in this way during HAZOP studies helps to increase the speed at which the report is produced, to reduce the man-hours expended in producing an agreed report and to minimize transcription errors. Lihou

claims that using the Hazop C programme he can produce, in a style suitable for all clients, a complete HAZOP study report within two days of the end of a study, (Lihou 1990). Other benefits that have been claimed for such tools are that they provide an inherent audit trail and good support for expediting actions, (Turner 1996). Turney emphasises the benefits of unambiguous records and claims that using computer recording systems results in more rapid completion of actions, (Turney 1991). There have however been concerns raised, (Ormond 1996), that the use of computer recording systems increases the temptation of adopting a mechanistic, check list, approach to HAZOP studies which runs the risk of stifling the creativity necessary for the process. On balance, for a HAZOP study carried out by an experienced team under the leadership of a suitably qualified chairman, such a use of computers can be seen to be highly beneficial.

8.4.2 Meeting support

Since the HAZOP technique came into use there have been a number of methods proposed to both make it more effective and to speed it up. Early efforts to address the first goal focused on the use of checklists.

Tolpa claims that the use of CAD workstation based 3D models of a plant helps HAZOP study teams to increase efficiency, reduce meeting times and record changes made during the meeting, (Tolpa 1994). In addition to using selected views of the plant to address points such as valve access the database associated with the model can be interrogated for information such as design pressures. The use of an on-screen P&IDs is also suggested with the ability to "yellow-off" lines that have been studied and note changes. One major draw-back to such an approach is the difficulty of a full review team being able to see information presented on a screen. Additionally, the ability to change a design during a study would have to be carefully monitored. It is not clear how the claimed advantages for this approach are achieved. Whilst the ready access to design information would be a benefit issues relating to layout form such a minor part of a HAZOP study that it is difficult to see how any major advantages could result from having this information available on screen. At the time in a project that HAZOP studies are carried out the layout is unlikely to have been developed to a level that would allow a 3D model showing detail such as valve position to be constructed.

Chung mentions a tool, QUEEN (QUalitative Effects ENgine), for the qualitative analysis of process plant behaviour that has the potential to be a HAZOP study aid, (Chung 1993). The paper does not make it clear how time consuming the system proposed would be to set up but the existence of a tool to predict the direction of change for a disturbance coupled with an ability, under development, to generate fault trees indicates that assistance in determining both the likely effect, and probability of, a disturbance could be provided. An application utilising QUEEN, called CHEQUER, developed by Rushton and co workers, (Rushton et al 1995b), is discussed in section 8.5.2.

Jones and Lihou mention a tool, CAFOS, aimed at aiding the performance and interpretation of operability studies, (Jones and Lihou 1986). CAFOS (Computer Aid For Operability Studies) depends on the generation of cause and symptom equations to construct fault trees and generate probabilities. Cause and symptom equations relate the deviant states to the events that cause them and result from them respectively. As described these equations must be generated by a study team but the use of expert rules applied to a computer simulation for this step is mentioned as a future development. Without such a step it is difficult to see how any benefit could be gained from the use of this tool. An additional draw back is the lack of two way propagation of process deviations.

Pitt and co workers report on the use of simulation tools to support the HAZOP study process and claim that a better understanding of, the increasingly complex, plants response to a deviation results, (Pitt et al 1995 and Pitt et al 1996). Any simulator could, in theory, be used but PRO/II and PROVISION were used in the work described. Whilst dynamic simulation would provide the best picture of plant behaviour it was claimed to be difficult to set-up. The quantity of information produced could also be difficult to interpret in a study situation. Thus the use of steady state simulation is proposed. Pitt and co workers developed a FORTRAN programme, Sim-Zop, to graphically represent the results of steady-state simulation runs before and after the application of a deviation. This approach, whilst providing an easy to interpret representation of the impact of the change requires a judgement to be made on the magnitude of abstract concepts e.g. how high is high pressure? If constraints, such as a vessel design pressure, are available an approach could be

to determine what magnitude of deviation causes the constraint to be violated. This could require more runs than envisaged in this work. Whilst use of a simulator within a review could be seen to be a potential hold up, access to qualitative data on impact would significantly reduce the time wasted due to discussions over opposing subjective views. Use outside the meeting could always be open to misuse by the person doing the simulation and would not be acceptable. Pitt and co workers claim that in addition to aiding understanding of plant behaviour the use of simulators would integrate environmental issues into HAZOP studies by providing mass balance data, (Pitt et al 1995). Emission limits could be set as constraints. This would be a great advantage as long as side reactions due to contaminants could be handled satisfactorily.

8.4.3 Expert assistance

Expert systems are well adapted to dealing with problems where there is no well established underlying theory but a body of knowledge that points in the direction of the answer. Early expert systems were developed in the field of medical diagnosis which clearly exhibits such characteristics, as do health and safety issues in process plants. Leading the field in this area were the Nuclear industry where early work is reviewed by (Baybutt 1986). CADET, an expert system based decision support tool concentrating on the safety of light water reactors, is described in more detail. Baybutt highlights the use of expert systems to assist in conducting analyses such as HAZOP studies as one of the areas where such systems could be applied to risk and safety management. Chae and co workers describe the development of a knowledge based expert system aimed at allowing designers to implement existing checklists and utilise past experience during HAZOP studies, (Chae et al 1992). They claim that the use of expert systems in HAZOP studies can reduce the manpower and time requirements necessary to carry out the studies. A reduction of more than 50% in manpower is suggested. Contained within the knowledge structure of the tool is information on equipment failures and material properties. The reasoning and rule networks allow this information to be utilised in both forward and backward chaining. Overall the knowledge base was designed to allow ease of future expansion. A major draw back of the system is the absence, due to difficulty of inclusion, of certain guide words: as well as, part of and other than. Reference

should also be made to Section 8.3 for a discussion of the ESPRIT STOPHAZ project aimed at developing a set of support tools for safety related design.

So far the implementation of expert systems has not been particularly successful due to the breadth and depth of knowledge used during HAZOP studies. The fundamental methodology of HAZOP studies is not knowledge based.

8.5 Automation of HAZOP Studies

The successful use of support tools has encouraged the examination of the process to identify if greater use of computers can be made in order to further lighten the HAZOP study load. A further incentive, as mentioned by (Rushton 1989), is that HAZOP studies are fundamentally an algorithmic application of rules which, given advances in the field of artificial intelligence, can be handled by available techniques. Rushton makes a distinction between computer tools that are supportive and designed to assist in the administrative aspects of HAZOP studies, such as HAZSEC, and those which are substitutive and designed to perform some of the hazard identification task. Automating the complete HAZOP study process would fall at the extreme end of the substitutive range and is viewed by some to represent the ultimate use of computers in this field.

Gillett warns that although computer systems can aid an experienced leader they cannot be regarded as a substitute for suitable training, (Gillett 1995), and this point is of particular relevance when considering automation. Four questions arise that must all have a positive response if such an approach is to ever be adopted in practise:

1. Is automation possible?
2. Is it necessary?
3. Is it desirable?
4. Is it safe?

Concentrating on the first of these questions initially. One of the first attempts at automation was carried out by Parmar and Lees who developed a rule-based system (Parmar and Lees 1987a) which was then applied to a water separator

system (Parmar and Lees 1987b). The method does not contain any means to address propagation of deviations through a plant and can only identify those causes and consequences directly related to the line under study. Subsequent work by Venkatasubramanian and Vaidhyanathan claims to have addressed the problem of propagation. They state that in addition to reducing the time and effort involved in a review an automated HAZOP study system can increase the detail covered by the review, and minimize or eliminate human errors (Venkatasubramanian and Vaidhyanathan 1994). These are sweeping claims that, if true, would indeed be strong arguments in the favour of adoption of an automated approach to HAZOP studies. An alternative approach to automated hazard identification and operability issues is adopted by (Dimitriadis et al 1996). Rather than automating the existing HAZOP technique they propose a model-based methodology for the verification and improvement of plant safety and operability. As HAZOP studies are not mentioned it is not clear if the approach is intended to complement or replace such studies. Complex models of a process are built and solved as an optimisation problem. The possible disturbances are the degrees of freedom, with the optimisation determining if any combination of values can drive the system outside predefined safety limits. Improvements are investigated by looking for values of the process and control system parameters that ensure operation within the limits even when the disturbance enters. The approach reduces safety and operability to a mathematical problem requiring extensive information for formulation of the models. During the early phases of design the required information would not be available making this only applicable to detailed design. Fundamental opportunities to achieve inherent safety would thus be missed. Recent attempts to develop automated HAZOP study tools are discussed in the following sections.

8.5.1 HAZOPExpert

A knowledge-based system called HAZOPExpert discussed by (Venkatasubramanian and Vaidhyanathan 1994) is based on dividing the knowledge used during HAZOP studies into general and process specific components. The general knowledge, called "process-general", is that which is likely to be used in a wide range of projects and relates to commonly occurring elements of plant such as valves, simple pumps and heat exchangers. The system architecture proposed has

general HAZOP study models of such items, referred to as units, and process specific information held within two separate, but interacting, parts of a knowledge base. Rather than attempting to automate the study of a complete plant Venkatasubramanian and Vaidhyanathan focus on the automation of the commonly occurring elements with the aim of freeing the experts to concentrate on the more complex and process specific elements. Using this approach, at least some control over the HAZOP study process remains with the team of experts. The process specific information, including the P&ID and data on the materials handled, must be entered by the user for each new plant that is considered. Although the method by which this data is entered is not specified and it is not clear if transfers from CAD and physical property systems would be possible, this activity has the potential to be very time consuming. Expending large numbers of hours preparing for a HAZOP study is simply shifting the effort and hours rather than reducing them and goes against one of the prime advantages claimed for automating HAZOP studies.

Venkatasubramanian and Vaidhyanathan of the Laboratory for Intelligent Process Systems at Purdue University have subsequently reported the results of a test comparing the output of HAZOPExpert with the product of a conventional HAZOP study given in (Lawley 1974). This test report does not include any information on the time taken to carry out the test and, although it is stated that all the causes and consequences identified in the original study were uncovered, no claims are made relating to increased detail or reduction in errors. Given that the list of deviations used is incomplete, both "reverse" and "other than" are missing, and the age of the study to which comparison is being made, there must be some doubt if the technique would fare so well if held up against the results of a HAZOP study carried out more recently. This would have the benefit of the experience and refinements resulting from many years of use. It should be noted that HAZOPExpert does not attempt to generate deviations automatically but relies on the user to specify them.

8.5.2 CHEQUER

Jefferson and co workers report on a tool called CHEQUER (Computer HAZOP Emulation using QUalitative Effects Reasoning), a HAZOP study driver linked to the QUEEN programme, (Jefferson et al 1995b). They focus solely on the hazard identification aspects of the HAZOP technique and so concentrate on the

design as it stands at the time of the study rather than attempting to make recommendations over changes, additions or deletions, that would result in an improved design product. As the determination of the need to generate actions to instigate such changes is the major objective of a HAZOP study the focus in developing CHEQUER severely under estimates the potential of the technique. Extensive follow up work would be needed to ensure that such actions were generated which, coupled with uncertainty over the time and effort required to produce a plant model suitable for use by the tools, places a question mark over the time advantage that would be gained over a conventional HAZOP study.

The proposed system is described as follows. QUEEN is used to build a signed directed graph (SDG) representation of the plant based on a model, source unspecified, and a library of standard plant units. As implemented only steady state, continuous unit operations can be handled and, whilst this is a major limitation the need to broaden the application to address unsteady state and batch operations is acknowledged. The ability to handle non-standard units must also be included. Whilst the paper does not address the preparation of a suitable plant model the use of the output from a simulation tool would result in the shortest possible lead time and, given a suitable simulator, allow a wide range of plant types and states to be handled. The SDG representation built by QUEEN is used to link process variables and determine the effect that a change in any variable has on any other within the plant. Only the direction, positive or negative, of the effect is determined and not the magnitude. This precludes any ability to rank hazards and allow the concentration of efforts on those that represent the greatest risk. Such an ability would greatly assist HAZOP studies by reducing the time wasted on detailed examination of issues with little overall impact. An example representation for a pipe is quoted but it is then stated that to model plants using QUEEN it is not necessary to include all the pipework. The model and hence the hazard identification is based on equipment items. This represents a major shift away from the line and equipment based emphasis of HAZOP studies and could lead to many important points, arising from items such as isolation valves, being missed. To be certain that all hazards had been identified it would be necessary to break down the plant in such a way that each pipe section between a potential blockage was dealt with separately.

Such a system would be cumbersome.

With CHEQUER it is claimed that a low level of decomposition will provide more detailed results than a high level but the reasons for this apparently counter intuitive statement are not given. The user selects the level of decomposition to be used before proceeding to select a port on the item to be studied. A series of guide words and deviations are then applied to this port. If each application were to require manual initiation, even with the limited range of guide word / parameter combinations given, this would be very time consuming.. The search method used by CHEQUER starts at a deviation and moves backwards until a cause, termed a fault, is identified. Consequences are then identified. There would appear to be no mechanism for forward cause searching which may result in elements being omitted.

CHEQUER applies filtering to the consequences identified to avoid duplication and to remove those where the consequence is not considered possible. Other than the use of physical properties to determine characteristics such as flammability how this filtering occurs is not clear. As noted previously some form of ranking would help determine if the consequences of a cause are significant or not.

8.5.3 Use of Expert Systems

A review of the use of expert systems in the safety area is given by (Rogers and Petry 1995) who include a report of a survey undertaken. 19 process related expert systems were reported ranging in size from 40 to 500 rules, 95 being the average. Development times ranged from two man months to eight man years. Topics were quite wide ranging covering design, eg relief calculation scenarios, training and operation, eg alarms management. Rogers and Petry discuss six tools in more detail:

(i) RATS (Risk Analysis Tool Set). Developed by Amoco to address a number of issues but focusing on the automation of process hazard analysis. The embedded APHA (Automated Process Hazard Analysis) programme implements API Recommended Practice 14C.

(ii) ADVENT. ADVENT was developed at Worcester Polytechnic Institute, USA, to facilitate the design of deflagration vents.

(iii) ENVIRO. ENVIRO was developed by Eastman Chemical to speed up the reporting of releases to atmosphere to the USA environmental agencies.

Using requested information a report is generated and e-mailed to the appropriate persons.

(iv) PHR-ES (Process Hazard Review-Expert System). PHR-ES was developed by Oxidental to guide review teams through the review process. Training, data handling and preparation assistance modules are included.

(v) EOP-SS (Emergency Operating Procedures Support System). EOP-SS was developed for the nuclear industry to train operators in the use of the emergency procedures.

(vi) HAZEXPERT. HAZEXPERT, developed at the University of Dortmund as an aid to the hazard analysis of P&IDs, focused on the early phases of design. The system can take DXF files as input, addressing concerns over set-up times.

A much more sweeping approach than that used by any of the tools discussed above is adopted by (Shimada et al 1994) who discussed the development of an expert system that would permit a lone engineer, possessing knowledge about the process, to perform the HAZOP study on a plant. Whilst this would undoubtedly result in a reduction in the cost of the study this approach raises serious questions about the quality of the results that would be obtained due to the complete absence of any team interaction. It should be noted that the list of deviations given by Shimada and coworkers does not contain "part of" which means that they will not be able to address situations where only part of the design intent is achieved. As with HAZOPExpert the knowledge base proposed is split into two parts, plant specific and generic, with the user required to input information on the P&ID and reactions into the former. Insufficient information is provided to judge if this would represent an onerous task. Generic knowledge is split into guide words, property words and decision tables. Property words are the process variables for items of equipment with a distinction drawn between manipulated and state variables. Decision tables give the possible relationships between input, internal and output states and are used for propagation. The case study used to illustrate the use of the tool developed is the Solvay Process for the production of sodium bicarbonate. When undertaking a study the user responds to a series of prompts, in the form of pick lists, that select the line,

property word and guide word to be utilised by the system. The results of a study are presented in the form of a record sheet that is in the form of a series of rather user unfriendly logic statements. No attempt is made to compare the results obtained with those obtained by the conventional technique therefore it is difficult to judge how successful the tool is at identifying all possible causes and consequences.

Zerkani and Rushton discuss a tool, HAZID, aimed at computer emulation of a HAZOP study, (Zerkani and Rushton 1992). Rather worryingly they state that the tool could be used by an engineer not skilled in HAZOP studies and claim as an advantage that the user is excluded from control of the generation of the cause / consequence chain. HAZID consists of a knowledge base, an inference engine, an evaluation facility and a masking facility. Information describing the plant has to be provided as a data file and, as pointed out by Zerkani and Rushton, without automatic generation of this file during the design this would act as a major hurdle to the acceptance of HAZID. A module referred to as HAZID is incorporated in the ESPRIT STOPHAZ project, (Preston and Richards 1995). Here the primary objective is not the elimination of a conventional HAZOP study but a reduction in time expended. There is no clear link to determine if the two systems have the same root. Bunn and Lees also mention HAZID during a discussion of the application of expert systems to plants handling hazardous materials, (Bunn and Lees 1988). They conclude that HAZOP studies have certain features that make it unsuitable for aiding by expert systems. These are related to the variety of knowledge types used and the breadth and depth of the knowledge. One area where expert systems could make a significant contribution is as prompts for hazard identification to "nudge" the HAZOP study team. Weatherill and Cameron also propose the use of expert systems to move towards a situation where a single engineer, familiar with the process, could carry out a HAZOP study, (Weatherill and Cameron 1989). The driving force again being to reduce the time and cost of HAZOP studies.

From the discussions above it would seem that, at least partial, automation of the HAZOP study process is possible, which answers the first of the questions posed at the beginning of this section. However the focus has been very much on hazard identification with little attention paid to operability or maintenance issues which are key to the success of HAZOP studies. Case study material presented by

Venkatasubramanian and Vaidhyanathan also appears to indicate that such techniques can identify the same causes and consequences as a conventional study going some way towards addressing the safety question. There are however still doubts over this point which rise considerably when systems are proposed that require only a single user. These doubts stem from the questionable ability of such a user to adequately identify and address points that fall outside their sphere of experience. The other two questions have, however, not been addressed as yet. Whether or not there is a need to automate HAZOP studies is partially answered by the fact that the process has received a degree of attention within the research community. However this can be viewed as driven more by the commonly held perception that there is a need to tackle the investment, time, effort and money, inherent in a traditional HAZOP study approach than by any conviction that this is the best way forward. As mentioned previously one of the most important aspects of a team based HAZOP study is the generation of ideas within a group of people of varying backgrounds. The leaps of logic involved are something that computers are not capable of and this is one of the prime arguments against the desirability of automating HAZOP studies. This conclusion is supported by (Kletz 1992) who in answer to the question "Could a computer carry out a HAZOP?" answers "Not for the foreseeable future". Two reasons are given. Firstly the inability of computers to adequately undertake a creative exercise such as a HAZOP study is highlighted. Secondly the difficulty that an expert system, necessary for automation, would have in handling all the different types of knowledge used in HAZOP studies is mentioned. Four types of knowledge are mentioned: plant specific, general process engineering, general scientific and everyday. Additionally a wide range of activities are undertaken during a study. Roach and Lees identify eight classes: selection of items for study, identification of deviation, generation of causes, generation of consequences, explanation of features, estimation of quantitative aspects, checks and specification of actions, (Roach and Lees 1981). Thus HAZOP studies can be viewed as a complex task where creativity is key, features that make it difficult, if not impossible, to automate. Rushton puts the case for increased computer emulation of HAZOP studies but falls short of predicting the redundancy of conventional HAZOP studies in the short term, (Rushton 1995). The argument for emulation hinges on the need to keep HAZOP

studies off the critical path of a project and no mention of quality, or indeed safety, is made. The impression gained is that emulation is a "nice" academic problem rather than actually giving any "real-world" benefits. Rushton concentrates on fault propagation in emulation for hazard identification but no mention of how operability, a key activity in HAZOP studies, would be addressed is made. The capture of sufficient problem specific knowledge is acknowledged as a shortcoming but highlighted as an active research field. No specific prototype systems are discussed by Rushton, although a general discussion of required prototype characteristics is included.

HAZEXPERT (HAZard Analysis EXPERT system) was developed to aid hazard analysis in process plant design based on P&IDs but not following the HAZOP study procedure, (Göring and Schecker 1993). Göring and Schecker claim that attempts to automate manual techniques, such as HAZOP studies, are not successful as significant sections of the methods are not knowledge based. HAZEXPERT is based on a top-down method of hazard analysis and as discussed only contains a generic data base concerning hazards that lead to dangerous over pressure. One feature of HAZEXPERT that is absent from other tools in this area is the inclusion of an interface, OFI, to a CAD system that extracts P&ID information on the process and converts it into a directed graph format. The requirement for P&ID level information precludes the use of the system during the early phases of design, as claimed to be possible by Göring and Schecker. HAZEXPERT can be used by a non-expert but produces a written report that can be evaluated by a expert prior to use in safety reviews.

8.6 Proposed Method

Having looked at the alternatives proposed to overcome the limitations inherent in traditional single stage HAZOP study procedure, the use of a staged approach appears to be both more feasible and desirable than the automation of the process. Elements of this latter approach should not be discarded, with the use of lessons-learnt databases and assistance in recording review discussions and actions showing the potential to give significant benefits.

8.6.1 Method Structure.

The main benefit of a staged HAZOP study procedure derives from the decomposition of a large, complex task into a series of more manageable sub-tasks, and as such a direct analogy can be drawn to the hierarchical design model proposed by Douglas and discussed in Chapter 4. Black and Ponton build on this analogy to propose a five level HAZOP study hierarchy, (Black and Ponton 1992), with each stage linked to a stage in the diagrammatic representation of the design. These are as follows:

1. Input-output block flow diagram. A very simple representation with the process as a black box showing main inflows and outflows only and no process equipment. Requires basic process and chemicals to be handled to be known.
2. Recycle block flow diagram. The basic black box developed to show the processing sections, for example reaction and separation, necessary for the plant and the major feed and product control loops. Account is taken of incomplete conversion and side reactions in drawing this up, requiring knowledge of feed compositions and reaction kinetics.
3. Un-integrated process flowsheet. A traditional process flow diagram showing the major plant items and control loops. The processing route must be essentially defined.
4. Energy integrated process flowsheet. As 3 but with a developed heat exchanger network.
5. Full engineering line diagram. The PFD developed to P&ID level to show all equipment and hardwired instrumentation.

At each of these stages a structured line-by-line study takes place with as many of the parameters and deviations listed in Table 2 being addressed as possible. During the early stages it is likely that questions will arise that cannot be answered unambiguously, therefore the generation of alternatives is inherent in the approach. The alternatives raised pass to the next stage to await the availability of sufficient information to allow a decision to be taken. Black and Ponton include case study material, based on the HDA process used by Douglas, that concentrates on levels 1 and 2 of their proposed structure but touches on level 3. At level 1 the only guide

word considered was Flow and no causes for the deviations were identified. All the actions raised related to the need to provide control measures. The addition of control loops resulting from these actions allowed Black and Ponton to revisit the study table initially produced and add causes relating to control valve failure. This approach results in heavy emphasis towards control issues at Level 1. Only partial results for level 2 are included by Black and Ponton but here it is possible to complete all the columns on the study table in one pass. Pressure as well as flow is considered. With the increased amount of stream definition available when moving to the un-integrated flowsheet the study at level 3 takes on more of the air of a conventional HAZOP study. Although reporting only part of the work undertaken at this level, Black and Ponton claim that the study allowed them to identify a number of potential operational problems and a fault in the published flowsheet for the process that results in a vessel having no means of pressure control or relief.

All five levels described above occur during the design, with Level 5 corresponding to a traditional HAZOP study, which represents additional reviews during this phase over existing staged techniques, discussed above. No post design phase reviews are included and these would be necessary to monitor the performance of the project during construction, commissioning and operating phases. To cover these phases adequately it is suggested that the five levels proposed by Black and Ponton be reinforced by the addition of levels 4, 5 and 6 of the ICI methodology described by (Turney 1990) and (Gillett 1995). This increases the number of levels to eight but extends the scope of the hierarchy to cover the whole of the life of a project. It should be noted that there is a mismatch between the method of determining the occurrence of levels between the two approaches. The ICI levels are fixed against stages in the life of a project, linked to obtaining expenditure sanction, whilst Black and Ponton fix their levels against design deliverables. As deliverables are directly linked to project stages this mismatch is not viewed as representing any difficulties in the combination proposed above. The eight level hierarchy proposed is shown in Table 4. This is fixed against key deliverables in the life of the project.

8.6.2 Case Study Work.

To demonstrate the use of the early stages of the proposed technique reviews of the HF case study work reported in Chapter 4 have been carried out using Levels

1 and 2 of the proposed methodology. The method of reporting adopted was to include only those points that lead to an action or a comment.

8.6.2.1 Level 1. Figures 1, 2 and 3 show the three block flow diagrams used as a basis for the level 1 study. These are marked up with the results of the study. Tables 5, 6 and 7 contain the study output for each of the blocks. Preliminary work based on Block 1 only is reported by (Black and Marsh 1995). It was found that two guide words, Flow and Composition, could be applied in turn to each of the lines entering and leaving the block flow diagrams. This expands the analysis undertaken by Black and Ponton and shifts the emphasis away from control. The actions raised were not limited to the provision of control measures but were split into actions, requiring a specific response and comments, prompts to pinpoint the need for further investigation. This split allows the recording of ideas generated during the study as flags for further investigation when more information becomes available. For example, during the study of Block 1 when considering the no flow case for the gaseous product a flag was raised to ensure that pressure relief requirements were considered at a latter stage in the design.

Following up the second action raised for Block 1, Line 2, Composition gave the typical sulphuric acid specification given below:

H_2SO_4	93.2 wt% Min.
S.G. @ 15.5 °C	1.835 to 1.837
Non-volatiles	0.02 to 0.03 wt% Max.
SO_2	40 to 80 ppm Max.
Iron	50 to 100 ppm Max.
Nitrate	5 to 20 ppm Max.

It was found to be quick and easy to undertake a Level 1 study. A low level of background knowledge of the process is required but by acting as a structured brain storming session surprisingly far reaching insights into inherent SHE can be achieved. Topics that were covered included the impact of impurities, control measures, relief requirements and separation scheme impact.

Blocks 1 and 2 gave identical results at this level and cannot the separated in the rankings called for in the design methodology discussed in Chapter 4. Due to the differences in feed materials used by Block 3 a separate table could be prepared in

this case but with a significant amount of overlap. The similarities in feedstocks used by the three blocks considered do not allow a meaningful ranking to be made.

8.6.1.2 Level 2. Figure 4 gives the marked up diagram used during the study and Table 8 gives the outcome of the Level 2 study. Study results relating to one feed line, line 1, one internal line, line 13, and one exit line, line 100, are included.

Line 1 is the fluorspar feed. This material is solid therefore the impact of variations in pressure can be ignored. The feed will be at ambient temperature and be subjected to climatic temperature variations. As long as the pre heat facilities are designed to cope with this then temperature does not have to be considered as a study parameter for this stream at this level. Flow and Composition are included in Table 8 for line 1.

Line 13 is the liquid phase acid stream from the gas treatment plant into the reactor. Temperature, Flow and Composition parameters are included in Table 8 for this stream. Pressure is not included as no sensible sources of pressure variation could be identified at this level,

Line 100 is the liquid HF product stream from the process. Pressure, Temperature, Flow and Composition parameters are included in Table 8 for this stream.

Some of the actions and comments included in Table 8 may appear to be stating the obvious but flags like this are needed to ensure that the obvious is not overlooked whilst tackling the more obscure but technically challenging design issues. One of the key actions to be raised during the study was the need to include a caustic scrubber on stream 100 to take the gas stream from the plant in case of a failure in acid supply. When undertaking the level 2 review it was found to be difficult to restrict discussions and prevent the time frame required from extending. Whilst this could be attributed to poor meeting discipline by the study leader, care should always be taken to avoid keeping such a tight rein that the creative process is dampened. Many of the apparent ramblings produced meaningful points for future consideration.

Due to time constraints only Option 3 was considered at this level therefore no ranking of alternatives, as required by the design methodology discussed in Chapter 4, is possible.

8.7 Conclusions

HAZOP studies represent a good technique for the systematic exploration of a design but, as currently used, the potential is under utilised. Operability issues, that should be included, are frequently over looked with a prime reason being the lack of suitable information and the lack of operating experience within many review teams. Adopting a staged approach allows issues to be incorporated into the methodology as soon as the required information becomes available and permits changes to be made to a design at a stage when the cost impact involved is minimised. To avoid a process that imposes a large burden of reviews on a design team then safety, operability, maintainability, construability, environmental impact and economics, the six success factors discussed in Chapter 4, should all be considered concurrently. Some moves towards the inclusion of environmental impact have already been made.

The automation of the HAZOP study process may, if knowledge capture problems are resolved, be a means of reducing the time spent undertaking reviews but in the near future it is likely to address hazard identification issues only. The breadth and depth of knowledge required to cover all the aspects required will remain outwith the capabilities of knowledge based systems for the foreseeable future. There is also a question mark over the advisability of attempting to automate a process where one of the key strengths are the leaps of logic that can be achieved by bringing together a group of people with diverse experiences.

The approach preferred here is to utilise a staged HAZOP study process that spreads the burden of reviews over the life of a project, splitting the work into manageable chunks. An eight stage approach that combines an established industrial six stage technique with an academic five stage technique has been proposed to address this need. The workings of the first two stages of the proposed technique have been demonstrated against the HF case study.

Table 1 - FAR for various activities and industries.

Activity / Industry	FAR
Clothing manufacture	0.15
Staying at home	3
Chemical industry	4
Travelling by train	5
Agriculture	10
Travelling by car	57
Travelling by air	240
Rock climbing	4000
Professional boxing	50000

Table 2 - Factors used in a traditional HAZOP study.

Parameters	Deviations	Description of Deviation
Flow	None	No part of intent is achieved but nothing else happens.
Temperature	Reverse	The opposite of the intent takes place.
Pressure	More of	A quantitative increase in a quantity, property etc.
Viscosity	Less of	A quantitative decrease in a quantity, property etc.
Composition	Part of	Only part of the intent is achieved.
	More Than	As well as the intent being achieved something additional occurs.
	Other Than	No part of the intent is achieved and something else occurs.

Table 3 - Six stage hazard study described by (Turney 1990) and (Gillett 1995).

Level	Purpose	When undertaken
1	To collect and review all of the relevant SHE information relating to the project.	Must be carried out as early in the life cycle of the project as possible if inherent SHE is to be achieved. Ideally during research and development.
2	To identify significant hazards and decide what to do about them.	Done during process and project definition. If it is done early enough can eliminate many SHE problems by reappraising the basic process.
3	As a traditional HAZOP.	Undertaken during the detailed design phase.
4	To check that the plant has been installed to the design specification and that it meets the statutory SHE requirements.	Carried out towards the end of the construction phase.
5	As 4 but with an additional check to ensure that measures to protect against physical hazards are present.	At the end of construction when a tour of the installation can take place.
6	To review operations, ensure that SHE criteria have been met, and check that all actions and documentation from the hazard studies have been completed.	After three to six months of beneficial production.

Table 4 - Proposed eight stage study procedure.

Level	Description	Purpose	Timing
1	Input-output block flow diagram.	Major material hazard identification. Aims to achieve inherent SHE.	Carried out during the feasibility study phase.
2	Recycle block flow diagram.	Major process hazard identification. Aims to achieve inherent SHE.	Early in the conceptual design phase.
3	Un-integrated process flowsheet.	Identification of changes to the basic process necessary to eliminate or limit SHE problems.	During the conceptual design phase when route options are still available.
4	Energy integrated flowsheet.	To check that energy integration for operability impact.	Early in the front end design phase.
5	Engineering line diagram.	Design check. To determine that the plant meets SHE criteria.	When the majority of the process design has been completed.
6	Installation review.	To check that the plant has been installed to the design specification.	Towards the end of the construction phase.
7	Site review.	To check that all the required safety measures are in place.	After construction has been completed.
8	Operations review.	To follow-up actions from preceding studies and review SHE performance.	After three to six months of beneficial operation.

Table 5
Hazard Study Table
Scheme : Block 1 (Stage 1 Study)

Line Number : 1
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow		No reaction	Comment: 1) Acid flow to be shut off on no solid feed.
More of	High flow		Unreacted Fluorspar in Calcium Sulphate	No hazard.
Less of	Low flow		Unreacted acid in Calcium Sulphate Reduced product	Action: 1) Neutral-ization facilities? - monitor acidity. No hazard.

Line Number : 1
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
Part of	More CaF_2		Either more HF or more CaF_2 in $CaSO_4$	No hazard
Part of	Less CaF_2		See below under more impurities	
Part of	Less impur ities			No hazard.
More than	More $CaCO_3$		Increased quantity of CO_2 produced	Comment: 2) Check impact on reaction scheme and product separation.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More SiO_2		Reduction in HF produced Increase in SiF_2 - a potential hazard	No hazard. Comment: as above Action: 2) QC on feed.
More than	More S		Increase in SO_2	Action: 3) Investigate route of SO_2 ie where will it come out ?
More than	More impurities		Increase in level of any/all of above	Action: 4) Investigate realistic limits.

Line Number : 2
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow		No reaction	Comment: 1) Likely to need flowmeter.
More of	High flow		See: Flow, Less of for Line 1	Comment: 2) Ratio control with fluorspar?
Less of	Low flow		See: Flow, More of for Line 1	

Line Number : 2
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
Part of	More water		Reduced amount of product. Potential corrosion problems below 70% acid	Action: 1) QC on feed.
Part of	More acid		Working in 93 - 99% region therefore unlikely to be a problem	
More than	More impurities			Action: 2) Investigate standard spec. of sulphuric acid.

Line Number : 100
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow		High level in liquid system or (high pressure in vapour system ?)	Comment: 1) Liquid inventory control system needed. 2) Consider pressure relief requirements.
More of	High flow	High reactant flow - either fluorspar or fluorspar and acid	Off spec. end product if separation system cannot cope	See: Lines 1 and 2.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
Less of	Low flow	Reduction in production	Reaction conditions non-optimal	
		Hold-up	High level / pressure (as above)	See above.

Line Number : 100
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
Part of				Not possible as anhydrous HF.
More than	Water impurity	Failure of separation train	Corrosion problems likely. Plant off-spec.	
More than	CO_2 and SO_2 impurity		See: Comp., Part of for Line 1	

Line Number : 200
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow	No feed		No hazard. Comment: 1) Would see problems in gas first.
		Hold up in plant		
More of	High flow	High flow of solids in	See: Flow, More of for Line 1	No hazard.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
Less of	Low flow	Low flow of solids in Partial blockage	See: Line 1	No hazard.

Line Number : 200
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More acid	High acid flow or low fluorspar flow	Disposal problem - neutralization See: Flow, Less of for Line 1	
More than	More HF			Action: 1) Consider if this is possible.
More than	More impurities			Comment: 2) Review in light of feed impurities.

Table 6
Hazard Study Table
Scheme : Block 2 (Stage 1 Study)

Line Number : All
Parameter : All

Guide Word	Deviation	Cause	Consequences	Actions/Comments
All				Comment: Refer to Block 1 results.

Table 7
Hazard Study Table
Scheme : Block 3 (Stage 1 Study)

Line Number : 1
Parameter : All

Guide Word	Deviation	Cause	Consequences	Actions/Comments
All				Comment: Refer to Block 1, Line 1.

Line Number : 2
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow		Reduction in reaction (assuming SO_3 and water still feeding)	No hazard.

Otherwise this line is as Block 1, Line 2.

Line Number : 3
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow		No acid formed resulting in dilution and temperature reduction. Worst case is no reaction. Neutralization unable to cope	Action: 1) If SO_3 flow stops water flow must be stopped.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More of	High flow		Would either: (i) Cause SO_3 break through into HF - impact? or (ii) Increase acidity in $CaSO_4$	Action: 2) Ratio control on SO_3 and water.
Less of	Low flow		Less acid formed. Dilution of acid. Possibly a reduced extent of reaction.	Action: As above.

Line Number : 3
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More impurities		Thought to be unlikely. Possibly air from ingress	Action: 3) QC on feed.

Line Number : 4
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow		No reaction leading to no acid formation and no heat release. Some SO_3 absorbed into acid but potential for break through	Action: See Flow, None for Line 3.
More of	High flow		Dilute acid. Possible thinning of slurry. Drop in temperature - reaction problems?	Action: See Flow, More of for Line 3.
Less of	Low flow		See: Flow, More of for Line 3	

Line Number : 4
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More impurities		Unlikely to be significant	Action: 1) Consider source and quality of water.

Line Number : 100
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More SO_3		Off-spec. material	Comment: 1) Check impact on product separation.

Otherwise this line is as Block 1, Line 100.

Line Number : 200
Parameter : All

Line is as Block 1, Line 200.

Table 8
Hazard Study Table
Scheme : Option 3 (Stage 2 Study)

Line Number : 1
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow	Blockage / failure of feed device	Effect on reactor heat load?	Action: 1) Shut-off all three acid based feeds when no flow of solids is detected. 2) Investigate means of detection of no solids flow eg motor stops, loss-in-weight system etc. 3) Consider effects of variable feed rate on reactor.
More of	High flow	Failure of feed rate control	Too much solid and waste of expensive raw material	No hazard. Comment: 1) How would this be noticed? Gross change may cause blockage but otherwise could depend on analysis of $CaSO_4$.
Less of	Low flow	Failure of feed rate control	Effect on reactor heat load?	Action: 4) Determine destination of excess acid.

Line Number : 1
Parameter : Composition

The feed is to be acid grade fluorspar therefore deviations in composition will be small. As part of quality and purchasing control procedures the composition of the feed material will be tested to determine suitability for use. Refer to Stage 1 study for background.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More water	Ingress of water during storage	Handling problems. Increased heat load on preheater	Action: 5) Ensure storage integrity is adequate.

Line Number : 13
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No flow	Failure of acid feed flow (Line 2) eg closed valve, pump failure etc.	HF heavily contamina-ted	Action: 1) Low flow alarm on Line 2. 2) LL flow trip to divert acid gas (Line 100) to a caustic scrubber.
		Blockage in line	High level in treatment plant	Action: 3) High level alarm and HH level trip on acid handling equipment.
		Acid heated above boiling point in gas treatment plant.	HF Heavily contamina-ted	Comment: 1) Temperature monitoring in gas treatment plant to be considered.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More of	High flow	High inlet flow	Excess of acid in the reactor leading to high levels of acid in reactor solid outlet and increased load on neutraliza-tion Handling problems and increased corrosion of reactor	Action: 4) Periodic sampling and lab analysis to be undertaken to determine pH of neutralization inlet and outlet streams. 5) Install a holding silo for solids discharge from neutralization for QA purposes. Action: 6) Install an inherent flow limit on the line eg low CV valve or ROP.
Less of	Low flow	Low inlet flow	Reduced quantity of HF if large drop Loss of fluorspar in $CaSO_4$	Comment: 2) Already have low flow alarm and LL flow trip on Line 2.

Line Number : 13
Parameter : Composition

The acid feed used will be commercial grade therefore the deviations in composition will be small. As part of quality and purchasing control procedures the composition of the feed material will be tested to determine suitability for use.

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More of	More heavi es	Material formed in the reactor that remains with the acid	Build up of material in the recycle loop with no route out of the process	Comment: 1) Consider the need for a purge stream.

Line Number : 100
Parameter : Temperature

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More of	High Temp.	Failure of condensing equipment in gas treatment plant	Either product too hot to handle or two phase flow or gaseous product	Action: 1) Temperature control to be included.
Less of	Low Temp.	As above	Only a problem if using chilled medium with the possibility of freezing	Comment: 1) Reconsider when condensing medium has been selected.

Line Number : 100
Parameter : Pressure

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More of	High Pressure	Increased driving force input	Stream is not fully condensed leading to two phase flow	Comment: 1) Pressure profile to be addressed during detailed design.
Less of	Low Pressure	High than expected pressure drop in gas treatment plant	May not have sufficient driving force to move material through the process	Comment: 2) As comment 1.

Line Number : 100
Parameter : Flow

Guide Word	Deviation	Cause	Consequences	Actions/Comments
None	No Flow	Blockage within process. Failure of reactants to plant.	As Hazard Study 1	
More of	High Flow	Failure of gas treatment plant. High reactant flow rate.	Off spec product.	Comment: 1) Design of gas treatment plant to capture possible variations in feed composition.
Less of	Low Flow	Partial blockage within process. Reduction in production.	As Hazard Study 1	

Line Number : 100
Parameter : Composition

Guide Word	Deviation	Cause	Consequences	Actions/Comments
More than	More impurities	Failure of gas treatment plant to achieve required separation	Off spec product	

FIGURE 1

01/08/94

Stage 1 HAZOP

BLOCK1

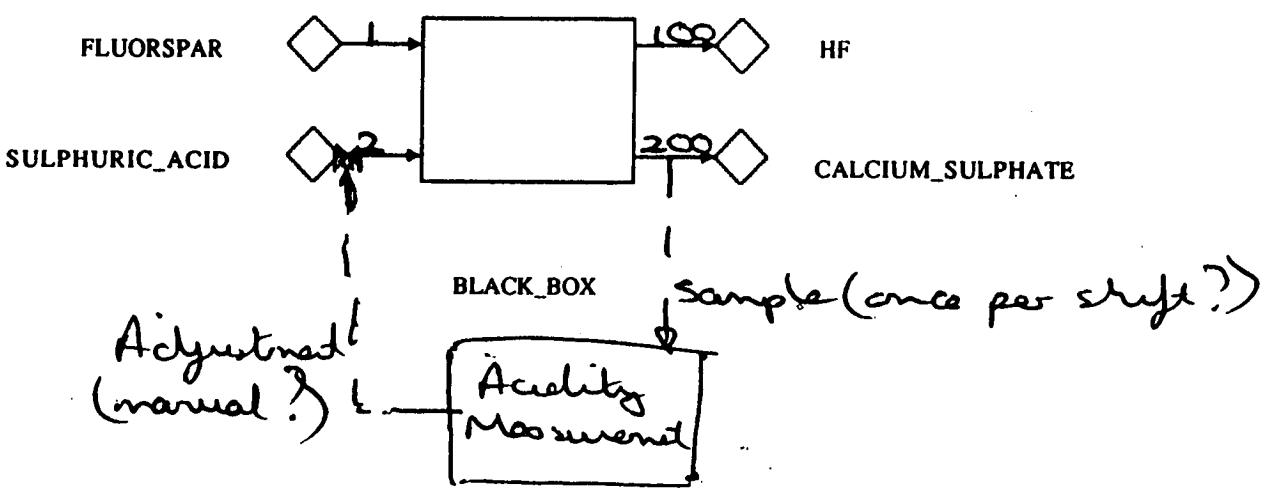
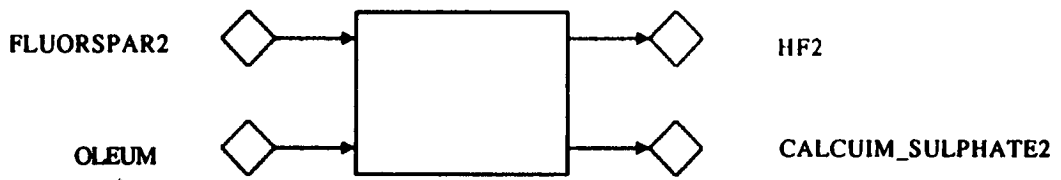


FIGURE 2

02/08/94
STAGE 1 HAZOP
see Block 1

BLOCK2



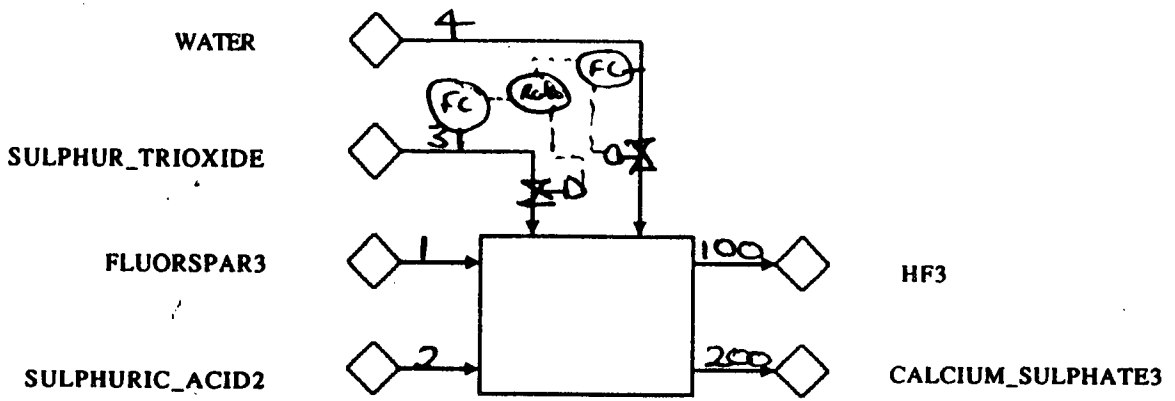
BLACK_BOX2

FIGURE 3

02/06/94

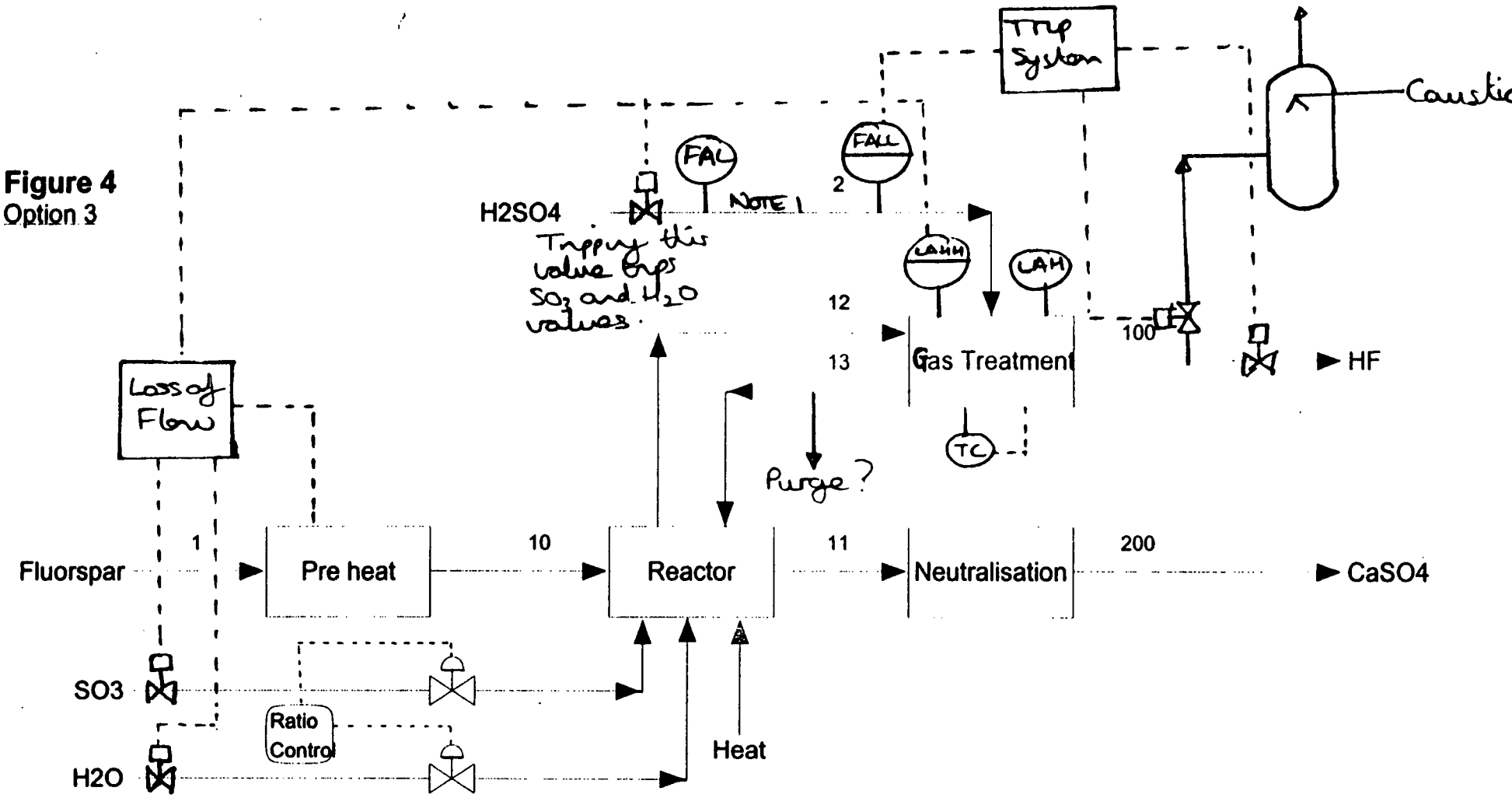
STAGE 1 HAZOP

BLOCK3



BLACK_BOX3

Figure 4
Option 3



NOTE 1
Limit flow to safe max. by low Cv valve or ROP.

Chapter 9

Conclusions

9.1 Introduction.

Before the wide-scale adoption of computers, the time taken to complete process engineering calculations manually limited the complexity of design problem that could be tackled and the number of design alternatives that could be explored. In freeing the engineer from the majority of number crunching tasks and allowing previously insoluble problems, such as dynamic simulations, to be deciphered the computer has been of great service; accordingly, the uptake of computers within the relatively short time since their introduction has been impressive. However, the increases in productivity that could have been expected have not been achieved and in some areas, eg process synthesis, designers have been very slow to adopt computer based research ideas as working tools. Whilst the failure of the computer to speed-up the work of the designer is partly attributable to the fact that it enlarges the range of alternative cases that can be examined, a more significant cause is the unproductive way that computers, and the data they produce, are at present being used. Too much time is still being wasted carrying out, in a rather haphazard way, mundane tasks such as pipework hydraulic checks which could easily be carried out in a more structured, semi-automated way. The consequences of using poor information handling procedures are exacerbated by the vastly increased volume of data that each engineer can now produce, so that the designer is almost swamped. Slow uptake of research tools can be largely attributed to two factors: a failure of researchers to take into account the wishes of the end user; and exaggerated claims for the capabilities and advantages of tools that are not borne out in practice.

There has been an increasing realisation that to obtain the best design product it is necessary to consider many factors simultaneously, particularly during the early phases of design, and to permit flexibility in support tools. The traditional focus on cost alone to drive design decisions is no longer acceptable. Safety, environmental performance and the ability to construct, maintain and operate the plant are also characteristics that must be designed in.

One danger associated with the increased use of computers is a developing dependency on the tools available, potentially leading to a "black box" mentality where the methods used by the tools are not questioned and the answers obtained are accepted as fact without questioning. This is exacerbated by the, cost driven, move away from in-house development of tools towards commercially available tools that allow users to produce "results" quickly but are not fully understood.

9.2 The Conflict.

At the centre of much of the ongoing work on the application of computers to process design is a conflict between those who see the way forward as dominated by the computer and those who see computers as tools that aid the designer but leave the important decisions to the user. The first set are advocates of tools that automate the design process to achieve cost savings by removing as many engineers as possible. Proponents of this view would, for example, advocate automating the hazard study process and allowing it to be carried out by a single person rather than a multi-disciplined team. Whilst this may be possible for discrete, well defined areas of design, such as the mechanical design of vee belt drives, it is questionable if it is achievable, or desirable, for complex systems such as chemical plants which rarely follow a set of predefined rules. The alternative approach is to acknowledge that humans, and their ability to make logic leaps, are essential to ensure a quality design product, leaving computers to aid the engineer by taking over those tasks to which humans are not so well suited. These are primarily related to the efficient handling of the large quantity of data generated during a design. AI has been the source of many of the tools and techniques used by this camp and it is likely that there will be further contributions from this field. The application of AI in design permits the understanding of how people reason about a problem to be used to develop intelligent aids to the design process. Knowledge based, or expert, systems are an example of an AI technique that has started to influence design methods. Constraint management, or truth maintenance, techniques are likely to become important in the future by flagging inconsistencies in a design to the user.

In all cases researchers have an optimistic view of the computing facilities that will be available to end users for the foreseeable future. Companies have invested

considerable effort and expense in PC based systems and are likely to show great inertia to a move to workstations or any other alternative. One of the finds of the questionnaire, Chapter 3, reinforces this opinion. This market survey was carried out with the aims of identifying user needs, looking at potential software and hardware platform limitations and gaining an understanding of existing user systems. It aimed at providing an interface between the developers and potential users of tools that could translate into a greater understanding between the two communities and, hopefully, lead to better design tools. 38 companies across a wide range of industries responded to the 82 questionnaires set out, a higher than expected response rate that indicates the importance attached by industry to this area. A total of 26 commercially available packages were included in the questionnaire or added by respondents. The most commonly mentioned were HYSIM (used by 44.7 % of respondents), ASPEN (39.5 %), PRO/II (31.6 %) and SpeedUp (also 31.6 %). On average 2.4 packages were named as being in use in each company. Software was mainly selected for the range of features offered (68.4 % of respondents) with price being a much less frequently stated factor. Industry is clearly prepared to pay for the "right" tool; it is also still prepared to spend the time and effort needed to develop in-house tools if no suitable commercial package could be found (61.3 % of respondents had done this). These in-house tools are generally for discrete, frequently occurring tasks (74.2 %) or for small, specialised design tasks (64.8 %). FORTRAN is the most common development language used (71.0 %). Spreadsheets are heavily used (by 76.3 % of respondents) but generally for simple, repetitive calculations. All respondents currently used PC's and most saw networked PC's, running Windows, as the future. Workstations were seen as becoming increasingly used, reflecting a shift away from mainframes and terminals. In line with the level of interest in consortiums such as PISTEP the most frequently mentioned desired additional feature was the ability to have a greater degree of integration between tools with the resultant improved data handling.

9.3 Hierarchical Methods

Two new hierarchical methods have been developed as part of this project, one a new model for the design process and one a modified staged hazard study

procedure. The early stages of these have been demonstrated as viable using a case study approach.

To develop tools to support the design process it is necessary to understand how an engineer would tackle a design. Of the existing models of this process the hierarchical, starting at an abstract level and adding successive levels of detail, is the most realistic. The basic five level Douglas hierarchical model is the most widely known of this type. There are, however, a number of drawbacks associated with this model. As well as a lack of generality, different models are presented to cover different design types, there is no linkage to project phase, poor exploration of alternatives, a focus on economics as the prime factor for making decisions, a reliance on design heuristics and a failure to incorporate heat integration until a late stage in the design. These short comings are illustrated by the application of the Douglas model to a case study, the manufacture of MEK from 2-Butanol. A seven level alternative hierarchical model is proposed to overcome the limitations of Douglas and the application of this model is illustrated using a case study based on the manufacture of HF.

Every human activity has an associated risk, commonly expressed as a fatal accident rate (FAR). The FAR for the chemical industry is quite low but this does not fit in with the public's perception of the risk posed. To minimise the risk and prevent accidents that tarnish the industry's image a key activity is the identification of the hazards associated with an activity / process. HAZOP studies have been a key tool in this area for a number of years. They have the great benefit of incorporating ideas generated from a team of various disciplines with a variety of background experiences, but tend to be time consuming and expensive, particularly if carried out only when final P&ID's are available. To counter this, staged, hierarchical, hazard study procedures have been in existence for some time. Other means of spreading the load that have been considered are providing support for the study process and automating it. A common problem with proposed staged approaches is that they tend to be concentrated on the later stages of design, at which fundamental design changes become expensive. An eight stage hierarchical approach to hazard studies is proposed to cover all the stages of a design evenly and overcome this limitation. This could be successfully linked with support tools that help record meetings,

discussions and actions. Attempts to automate the hazard study process are seen as undesirable and potentially dangerous. Costs may be cut, but at the price of potentially unsafe situations arising due to the lack of ability to draw on diverse experiences.

9.4 Use of Novel Design Tools

Three novel design tools developed at Edinburgh University, CHiPS, KBDS and épée, were used as part of this project. This aspect was not particularly successful for a number of reasons. Of the three, the use of épée was the most disappointing as the use of integrated environments is seen as key to the future development of process engineering. Many of the failings can be attributed to difficulties in setting up a realistic test case within an academic environment. In particular, it is difficult to simulate the commercial pressures that apply and to have the same quantity of background information available. Using the tools during an actual design is necessary to give an accurate evaluation of their capabilities.

CHiPS is a process synthesis tool which aims to service the step in design where the components of the plant are selected and interconnected. A number of alternative flowsheets are generated, and these are ranked with respect to economical efficiency and environmental acceptability. This can be done, either for whole processes or for separation sequences only, with or without heat integration. CHiPS could not be used for the HF case study used elsewhere as it could not handle solids, but was tested against the MEK from 2-Butanol case study. It proved to be difficult to set up and run without the help of the developers, mainly due to the poor level of on screen help and manual availability. CHiPS requires interfaces that are more user friendly than those provided, applicability to a wider range of unit operations and the ability to cover the transition into more detailed design phases before it can move forward towards main stream acceptance.

KBDS attempts to address a pressing concern, the recording of an auditable design history showing the evolution of a design. Issues of choice appear during a design due to the inability to provide definitive answers to questions that arise. To each issue there correspond positions that can be adopted and arguments that support / counter these positions. These three elements, issues, positions and arguments,

form the basis of the IBIS representation used by KBDS as the basis of the design constraints and specification network. Two other networks, design alternatives and models of these alternatives complete the KBDS representation of design history. When using KBDS it was found to be far from robust, with a disconcerting tendency to crash and loose considerable chunks of work. A key element of KBDS, truth maintenance, was unavailable for testing during case study work but the intent tool, a significant novel feature, was found to be easily usable. KBDS shows promise as a tool to fill an obvious gap in the market.

Épée was developed to address a perceived need to cover the sharing of information between design tools. It is an integrated design environment. At the time of testing, limited links to applications were available making it difficult to judge the potential of the system. Épée was found to be difficult to navigate around but was robust and rarely crashed. It suffered from the opposite problem to KBDS, with an excessive amount of information saved; this would lead to problems in sorting and use when undertaking a design. Integrated environments are key to the future of process design but must be user friendly.

9.5 Wish-list

To help me to look towards the future of provision of design tools, I constructed the wish-list given below. This addresses frustrations that I have encountered whilst undertaking design work.

1) The alternatives explored during the design of a plant should be recorded in a form that allows a) backtracking if a selected path proves to be unfeasible, and b) for the subsequent exploration of promising alternatives which time constraints prevented being exploited fully at their first appearance.

2) On-line expert systems should be provided to aid the engineer carry out tasks such as physical property data determination and equipment type selection.

3) A design support system should include: multitasking to avoid wasting time waiting for applications to run; on-screen help, to avoid the need to frequently refer to manuals; manuals that are well indexed; and the systems should be robust, so that user errors such as problems with mouse control do not cause the system to crash. Automatic saving of work is essential, to avoid the frustration caused by loss of data

and to allow the user to take steps backwards to recover from errors.

4) By using a design support system the engineer should be freed from much of the data handling that has traditionally taken-up so much time during the design process. Database technology is a key element of any integrated engineering system designed to address this point but for any database to be effective there needs to be a good understanding of the relationships between data and how it is exploited. Particular attention should be paid to the generation of output reports in an concise format that is readily utilised. Initiatives such as PISTEP, aimed at electronic transfer between tools represent a major step forward in data handling.

5) All design tools and their associated literature should avoid the use of computer jargon and be written in terms of the engineering language readily understood by potential users.

6) The user should be presented with a well designed, standard GUI for all applications used, minimising the learning curve for each tool.

7) Specification sheets should act as GUIs to the work that has gone into preparing them. Each item included should be a window to the design history that produced it. This history could be text describing assumptions made and reasons for decisions taken or calculations. The situation where an extensive paper trail, with a high probability of gaps, is required to determine why a design element is as stated is inefficient and wasteful, as is the need for reams of handwritten calculations to be checked and approved separately from the specification sheet they refer to.

8) There should be a method of linking operating instructions and plant drawings, such as P&IDs and isometrics, with a plant design database in such a way that when modifications are made to the design a flag to modify the affected documentation is raised. All such changes must be fully recorded to give a complete design history of a plant.

9.6 Pointers for the Future Direction of Research

Researchers need to bear in mind what the target end users want. There will be little uptake for elegant mathematical tools that are difficult to use. An ongoing dialogue between the two communities is vital.

Design tools must not replace the questioning aspects of human intelligence

but must support users by freeing them of mundane tasks and allowing them more time to think. Such tools must be easy to use but with limitations clearly flagged to the user.

The electronic exchange of information between tools must be exploited fully to avoid the need for manual transcription, with the attendant risk of errors.

Increased exploration of expert systems to provide support to the designer should be explored fully - for example, by providing input on previous incidents to a hazard study team.

Footnote

In almost all of the research papers reviewed during this work the people undertaking process design were referred to by titles other than engineer. Does this reflect a view that the engineer can no longer be expected to be innovative?

Chapter 10

Glossary

10.1 Terminology

Variations in terminology are prevalent across the field of process design. The specific meanings of terms as used within this thesis are detailed below.

"*Process Design*" This covers the whole range of design activities normally undertaken by a chemical engineer from the development of the process flowscheme to the detailed design of individual equipment items. The process referred to here follows the classical chemical engineering definition of a series of unit operations performing some chemical and / or physical manipulation.

"*Conceptual Process Design*" As discussed above the term "*process design*" covers a range of design activities whereas the addition of "*conceptual*" to this term indicates a much narrower focus. Conceptual process design covers the design activities that commence with a blank piece of paper and on design objective and end with the production of PFD level information on one or more processes. Covers phases 1 and 2 of the structure defined earlier in this chapter.

"*Design Process*" This describes the method by which design is tackled ie the route from the blank piece of paper to a completed, functioning object. This object may be a chemical plant but it could equally be any product that is designed from a paper clip to a space station.

"*Process Synthesis*" This refers to the generation of possible processing schemes based on some minimal level of specification information. Generally this term can be taken to imply the use of some form of computer tool to undertake the generation and to produce more than one alternative. However it could equally well apply to manual alternative generation.

"*Process Simulation*" This refers to the step in the design process following process synthesis where the operation of the unit operation structure is modelled. This normally occurs by the application of one of the commercially available software tools. Traditionally this would have required extensive manual calculations and the speeding up of this step has been, to date, one of the prime advantages of the

use of computers in process design.

"Project Specification" Whereas the term *"process"* refers to the definition of a plant in the language of chemical engineering (i.e. as a series of interlinked unit operations), the use of *"project"* refers to the multi-discipline terminology used in the effort required to realise the plant as a functioning entity. The project specification is thus the document that defines the plant using such terminology and includes the information necessary allow the multi-discipline term to progress the work necessary.

10.2 Abbreviations.

The following list defines the abbreviations used throughout this thesis.

AI - Artificial Intelligence. The branch of computer science aimed at developing computer systems that exhibit some of the intelligence characteristics of human beings.

BPEO - Best Practicable Environmental Option. For industries that give rise to the most serious pollution problems or have the greatest potential for multimedia pollution the processes operated are designated as Part A processes under the Environmental Protection Act 1990. For these processes the overall impact on the environment must be considered with the aim being to achieve the BPEO.

BATNEEC - Best Available Techniques Not Entailing Excessive Cost. A concept introduced by the Environmental Protection Act of 1990 that requires the use of technology, design and operating practises to prevent or, if this is not possible, minimise, pollution to the whole of the environment.

CAD - Computer Aided Drafting. The use of one of a number of commercially available tools to prepare drawings such as P&IDs. The term is used by some sources to refer to computer aided design but this usage covers too wide a range of applications to have any real meaning.

DBMS - Data Base Management System. A set of interrelated software tools to construct and maintain a database.

FAR - Fatal Accident Rate. Previously known as Fatal Accident Frequency Rate (FAFR). The number of fatalities per 10^8 hours associated with undertaking a particular activity.

GUI - Graphical User Interface. A front that allows the user easy access to

programmes within their environment using mouse operations, point and click, rather that commands in the operating system language. The presence of an application is represented by an icon.

HAZOP - Hazard and Operability Study. A technique for addressing the hazard and operability aspects of design by undertaking a line by line analysis of P&ID's.

HEN - Heat Exchanger Network. The arrangement of interconnected heat exchangers that results from the application of heat integration to a plant.

HMIP - Her Majesty's Inspectorate of Pollution. UK government department responsible for policing the Environmental Protection Act, 1990. As of April 1996 this function was incorporated into the role of the newly formed Environment Agencies, one covering Scotland and one the rest of the UK.

HSE - Health and Safety Executive. UK government agency responsible for policing health and safety legislation.

IPC - Integrated Pollution Control. Concept introduced by the Environmental Protection Act 1990 and requiring processes to consider releases to land, air and water as a whole. Aim at avoiding the transfer of pollution from one medium to another.

KBES - Knowledge Based Expert System. A tool containing a domain specific knowledge base and inference engine for use to automate reasoning about a system.

LAN - Local Area Network. A network designed to provide facilities for non-voice inter-user communication within a single geographical location.

MINLP - Mixed-Integer Nonlinear Programming. Solution technique used in tackling large non-trivial synthesis and simulation tasks.

PFD - Process Flow Diagram. Simplified representation of a plant showing the major items of process equipment, their interconnections and control loops.

P&ID - Piping and Instrumentation Diagram. Also referred to as Engineering Line Diagram (ELD). Shows all items of equipment, lines, instrumentation and controls. Developed during detailed design and used as a basis for conventional HAZOP studies.

SHE - Safety, Health and Environmental. Usually applied to standards etc

that must be meet by any project to ensure that the impact on people, operators and the general public, and the environment is within acceptable parameters.

STEP - Standard for the Exchange of Product model data. An emerging standard to allow communication between software produced by different vendors.

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