Multi-Objective Process Synthesis And A Post Synthesis Environment For Process Design

Greville Wade Williams

Thesis Presented for the Degree of Doctor of Philosophy

University of Edinburgh

2000

Declaration

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

Acknowledgements

I would like to thank the following people and organisations for their assistance and support throughout the course of this study.

Professor Jack Ponton for his supervision and guidance throughout this work. Dr Eric Fraga for his advice, especially at the start of the project. Ross Andrews for his help programming and creating a framework of web objects.

I would also like to thank all my friends and work colleagues in the department of chemical engineering for their advice and support.

The Engineering and Physical Research Council for providing the funding. Edinburgh University for providing the infrastructure for this project.

I would especially like to thank my family for their love and support over a long period of time without which this project would not of been possible.

Finally I would like to thank Jane Munro whose love has meant so much over the past few years.

coda /’kəʊdə/**n** **1** *Mus* the concluding passage of a piece or movement, usu. forming an addition to basic structure. **2** *Ballet* the concluding section of a dance. **3** a concluding event or series of events. [It.f.L *cauda* tail]

`The Oxford English Dictionary`

Abstract

This thesis describes a process design procedure incorporating early consideration of extra design criteria. Traditionally cost is used as the main criterion to select a design alternative, but the design specification frequently has approximations and uncertainties associated with it. Further criteria for evaluating processes can be used to help the designer differentiate between alternatives.

Synthesis is carried out on a cost basis selecting the n best processes based upon cost. The synthesis output is reassessed on the grounds of safety, environmental impact, flexibility etc. The procedure is applicable to conceptual design and forms the basis of further analysis. Where transparency and flexibility is required in the analysis, external packages are used.

A post synthesis environment is described which stores the extra data required to perform the procedure and enables a collection of processes to be examined. Relationship assessments and value based assessments are applied to conflicting criteria so that a process ranking can be made.

The procedure has been applied to two case studies in the manufacture of hydrogen cyanide and ethylene. The studies show how the method can be applied and demonstrates that the design selected upon a cost basis alone may not be the optimal design. The procedure demonstrates the requirement that the assessment package and synthesis package are linked to ensure consistency of the data set, and a record of all previous data sets are maintained. The cost of incorporating inherent features into a design can be evaluated and inferior designs can be removed from further consideration. By assessing the process alternatives early on in the design, development time can be reduced and the designers attention can focus upon the best process alternatives.

Contents

List of Figures

List of Tables

Chapter 1

Introduction

Chemical engineering is the process of designing, constructing and operating chemical process systems and it is the aim of the chemical engineer involved in design to achieve the best design possible. Fundamental to developing a process design are the decision making steps that an engineer has to make, for which design methods exist to help the designer make informed and rational choices. This work examines the systematic design methods available and shows how a broader design method can be used.

The process of designing a chemical plant is well researched as are the individual methods employed to help an engineer design a new chemical plant. Most of these design strategies for process synthesis[1] focus upon cost, and obtaining the most profitable design. However, with so many potential options available few of these designs become commercially successful due to unforeseen complications with the design. Reducing the number of design alternatives early on is essential since cost escalates as the design proceeds and market pressures insist that a new product is delivered quickly and efficiently. It is therefore becoming more desirable to evaluate of all issues associated with design as soon as possible.

The economics of a process is the primary driving force behind synthesis and usually the design task has been to optimise the profit of a process. Further operating criteria placed upon the process rarely mean that the most financially profitable process can

---

[1] Process synthesis is the selection of equipment and interconnections to achieve a certain goal.

be chosen without further justification. This can be seen through time where processes have gradually had to deal with tighter restrictions upon other criteria. In the 1960's, due to a number of high profile losses, safety became a major concern. In the 1970's energy consumption became a critical factor and in the 1980's control and flexibility gained increased importance with the demand for high specification products. In the 1990's concern for the environment brought about a wide range of environmental issues that had to be assessed. For a successful design to be implemented it has to satisfy all of these criteria and still be economically viable.

The design of a chemical process can take a long time with a number of different teams working on a part of the project. Therefore the design procedure needs to promote communication between design teams, record the decisions taken and still allow for creative input. Figure 1.1 shows how the design process can progress from project concept to detailed process design. The post synthesis analysis procedure covers the area from the generation of the process structures through to the point where detailed design in carried out.

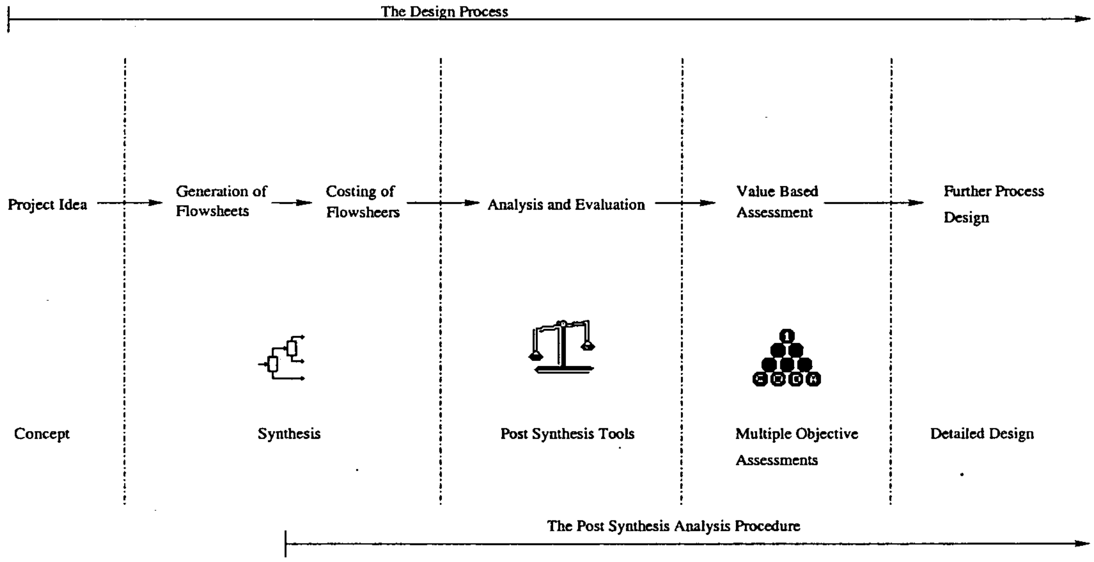


Figure 1.1: The Design Process

The work presented in this thesis approaches the problem of assessing conceptual designs early on in the design process. The aim of this work is to identify and exploit inherent benefits within competing designs so that better process can be built. Post-synthesis analysis is the analysis method by which a set of conceptual level processes are examined and their characteristics evaluated. The analysis is aimed as a guide to assist the designer and is not intended to remove creative input, but rather help the designer examine different alternatives and justify the decisions taken. It is intended to give indications about potential problems and improvements that can be made to the system. Conceptual design should not only be the foundation for designing the final process flowsheet but should also be the start of assessments made about the design. It is therefore desirable that further study should follow a similar format of analysis as that used at the conceptual level. This should then gives the ability to track any errors back to the analysis stage.

With an increase of the computational power available to a designer the conventional methods of synthesis can be re-examined. A depth first search where one design is examined in detail can be replaced by a much broader search of all alternatives. The implications of these alternatives needs to be explored so that the best process designs can be taken forward for further consideration.

The large number of assessment and simulation tools potentially available to the designer can return an overwhelming amount of information to the user. This requires methods that highlight the important features of a design and help the designer make effective judgement trade-offs. Design is a team activity and communication between people is essential if the best designs are to be considered. This then requires a recorded knowledge of what has been examined and the respective conclusions.

This thesis proposes a method where a range of processes can be analysed. Conflicting criteria require a method which can select the best process alternatives. Only if the situation is obvious, where a process excels in all areas, can the design be confidently progressed further, otherwise a value based judgement has to be made. This work presents a method by which different processes can be assessed, judged against each other and where applicable taken forwards for further design.

There is a gap in the knowledge between the point where a design is developed and the assessment tools applied. Some design synthesis strategies develop a single detailed design to which further assessment methods can be applied, while other synthesis strategies are much broader with less detail associated with them. Therefore not all assessment methods are applicable to each synthesis strategy. Previous work has mainly focused upon the synthesis stage for a particular purpose or upon the analysis stage of design. Ideally, a combination of synthesis and analysis tools should be used.

This thesis contains a number of reviews of previous work in different chapters. Chapter 2 contains a review of the synthesis methods available and their limitations. Chapter 4 covers some of the main assessment tools available, and shows how they can be applied to a design strategy. Connecting the synthesis methods to assessment methods requires a data management system discussed in chapter 3. Alternative data management systems are discussed, and a post synthesis environment is proposed. Chapter 5 reviews some of the methods of decision making where multiple objectives have to be satisfied. This enables judgements to be made where there is conflicting criteria. Finally, the developed analysis technique is applied to a hydrogen cyanide case study in chapter 6 and an ethylene case study in chapter 7.

Chapter 2

Synthesis

The search for a systematic procedure for conceptual design of a chemical process has been extensively studied with a number of different approaches proposed. The four techniques of synthesis is reviewed by Hendry and Rudd [1] and the systematic method of chemical process design reviewed by Biegler et al.[2]. The most practised technique is used by Douglas [3] is the heuristic approach to synthesis. The method uses a combination of shortcut calculations to screen alternatives and cost studies to eliminate unprofitable designs. Only if a process appears to be financially profitable are other factors such as safety and environmental constraints considered. The main benefit of this approach is that it leaves the designer free for creative thought applying appropriate technology wherever it is required. However, it fails to search the entire design space for the best alternatives and a more formalised approach may be required.

Processes synthesis can also be decomposed using a method described by Rudd[4] from the input/output structure. The processes are gradually decomposed until technologies exist which are capable of producing the required system. In general a branch and bound approach is taken utilising different technologies until a solution is found. Bounds placed upon the search have been developed by Daichendt and Grossmann [5] to eliminate unfavourable alternatives early on in the design.

Synthesis can also be carried out by applying an algorithmic procedure to find the optimal operating conditions for a system. Knowledge of all possible flowsheets is required and are overlaid upon one another. An algorithm is then applied which is able to select the best combination of processes.

The final method to synthesis of a new plant is to examine what has been done before and take an evolutionary approach to synthesis. Examining how things could have been done better and applying those findings to a new design should lead to an improved design.

2.1 Synthesis Methods

2.1.1 Process Design Decomposition and Branch and Bound Strategy

Process Design Decomposition was first described by Rudd [4] where a design problem is broken down into sub problems until technology exists to solve each component part. The method requires that the user specify the system performance and the technologies that can be used.

The main advantage of Process Design Decomposition is that it provides the framework for the systematic synthesis of quite large general design problems. However it is difficult to ensure that an optimal solution has been returned as it is dependent upon how the system has been decomposed. This has been shown by Papoulias and Grossmann [6] with the structural decomposition of a utility system where the optimal solution of a set of sub-problems is not the global optimal solution.

Methods to decompose a system systematically involve breaking the problem into loosely coupled sub-problems which are assumed to be independent. Hendry and Huges [7] have demonstrated how an exclusive task enumeration technique can be applied over every set of possible separators. The first stage is to evaluate all two component separations and evaluate their cost. For example a system with five components A,B,C,D,E requires the cost of the following separations to be evaluated:

$$\frac{A}{B'}, \frac{B'}{C'}, \frac{C'}{D'}, \frac{D'}{E}$$

Where the superscript indicates components above or below the split point.

Then the generation of all three-component separations follows and is costed. For a three component system the cost from the first separation is known and the entire cost of the system evaluated. This method can be expanded for any number of components and other process operations.

Johns and Romero [8] proposed an automated method using an implicit enumeration procedure to carry out a branch and bound technique with primal and dual bounds, and dynamic programming. Computation of a process flowsheet starts with a given feed stream and generates a flowsheet by working forwards until all outlet streams are acceptable process outlets. The dynamic programming allows the system to obtain the best cost for each unit and the bounding technique enables the search to focus on the most profitable alternatives. This method of searching is only suitable for an acyclic structure.

Methods to include cyclic structures have to reduce the search space and a discretisation method has been employed by Fraga [9] in the creation of process synthesis package CHiPS. CHiPS is a package for the automatic generation of process flowsheets incorporating heat integration at the initial design stage. The search is carried out to find the minimum cost of units along with the profits generated by the product streams. Finding the optimal solution requires searching over continuous space which can give the possibility of an infinite search space. The CHiPS method of synthesis overcomes this problem by discretising the component flows, heat exchange quantities and stream enthalpies. Structures of processes are analysed and the best processes alternatives returned. On of the main advantages of this method is the ability to return multiple structures which can form the basis of further design.

2.1.2 Hierarchical and Heuristic Approach

A hierarchical approach gradually decomposes a problem from the input-output structure by progressively adding more detail. This common sense approach has traditionally been used by the chemical industry. The Hierarchical approach requires evaluation of the best alternatives at each level of design and is most often used with heuristics. A heuristic rule is one that seeks a solution to a problem by means of plausible but fallible guesses.

This combination of hierarchical and heuristic approach to chemical process design is best described by Douglas [3] and a computational approach is given by Lu and

Motard [10]. The design is broken down into five levels from the choice of a batch or continuous process through the input-output structure, recycles, separation system and heat exchange system. Many of the heuristic rules and rules of thumb have been gained through experience and in many cases represent common-sense decisions. For example the general heuristics for column sequencing.

1. Remove corrosive components as soon as possible
2. Remove reactive components or monomers as soon as possible
3. Remove products as distillates
4. Remove recycle streams as distillates, particularly if the are recycled to a packed bed reactor.

The reasoning behind these sets of rules is not entirely based upon cost alone. For example the removal of corrosive components is cost based so as to facilitate the use of carbon steel. Where as the removal of reactive components early on is recommended to simplify the separation sequence and prevent the reboiler from becoming fouled.

The heuristic method can lead to failure of the design as the guesses fail to predict all of the necessary interactions. It is quite probable that sets of rules will contradict each other due to the fact that they cover only a limited domain of problems.

The hierarchical approach leads to a 'depth-first' search which contains a lot of detail about the process being synthesised, and enables the design team to identify problems quickly. A flaw with this approach is that design decisions taken early on influence later design and the optimal design may not be chosen.

2.1.3 Direct Optimisation

Direct optimisation requires that all possible flowsheets are known and then overlayed on top of one another. The method involves embedding all the interconnections which might exist between pieces of equipment or systems of equipment into one model. This is referred to as a superstructure and the problem is defined as a mixed integer linear program (MILP), or mixed integer nonlinear program (MINLP).

Grossmann [11] [12] and his students have dominated the research in this area. This method selects a single plant design by eliminating redundant unit operations and selecting optimal operating conditions. The main problem with this method is generating a general flow sheet which incorporates all possible flowsheets. If the designer wants to examine sub-optimal flowsheets the optimal flowsheet must be removed from the superstructure. Examples of applying this technique have been made to heat exchanger networks (Floudas et al [13]), separation sequences (Floudas [14]) and entire process flowsheets (Kocis and Grossmann [15]).

2.1.4 Evolutionary

Evolutionary synthesis refers to the synthesis of a new process by modification of previously generated processes or part processes. It is probably the most commonly used and best understood method of synthesis. The method involves taking an existing design and modifying it when a new system is required. The obvious problem of the evolutionary approach is that it relies upon an existing design and if that design is fundamentally sub-optimal all subsequent designs will be flawed.

It can also be used to improve a process design developed by one of the other three methods. Some cases of evolutionary design utilise target setting. For example most heat exchange networks are designed using the 'Pinch' method developed by Cerda et al [16] where the target is to reduce energy consumption down to the minimum utility load.

2.2 Synthesis with Multiple Criteria

Each of the methods discussed have their own advantages and disadvantages, and this becomes more apparent when multiple criteria are introduced. As more emphasis is placed upon other criteria such as safety and environmental impact cost becomes less of a decision making incentive. A few approaches have tried to combine multiple criteria explicitly in the search for a process design but all of them utilise one of the described synthesis strategies.

The heuristic and hierarchy method has been developed over time by trial and error to satisfy a number of different criteria. Rules have been written into the design in order to achieve a working process. Many of the rules have practical reasons for their existence and not always based upon cost. However, it is difficult to quantify some of these rules and their existence can become entrenched in design thinking. The heuristic approach can be expanded and Padley [17] has incorporated operability measures into process synthesis using a hierarchical approach.

Evolutionary design is most successful when a degree of fitness test exists for each process. For heat exchange networks this can be expressed as how close the system gets to the minimum utility requirements and the cost associated with the required heat exchangers. For criteria where limits to improvement do not exist such as the environmental impact and safety it is difficult to quantify a target for the system. In these cases evolutionary improvement may not be the most appropriate method to advance the design.

Direct Optimisation is only capable of finding the optimum for one criteria which is normally cost. Unless other criteria can be expressed in terms of cost then direct optimisation will be unable to find the best solution. For example unless environmental impact can be quantified along with safety in terms of cost then the system is unable to find the multi-objective solution.

Branch and bound techniques have the advantage that they search a much wider search space with the possibility of generating structurally different flowsheets. Similar to direct optimisation unless the value function is known the synthesis stage is not capable of performing a multi-objective search. Bogle et al. [18] has tackled this problem for environmental problems by using the land area required to achieve a sustainable process. If a value function can not be generated then the generated solutions have to be analysed and re-evaluated accordingly. The main advantage branch and bound has over other methods is it's ability to generate multiple flowsheets which can in turn be analysed on the grounds of other criteria.

Chapter 3

Post Synthesis Environment

In order to assess the viability of a design requires knowledge of the process data. There are two suitable methods of handling this information. Writing an object oriented analysis tool is one possibility, where data is stored in objects and referred to for analysis when required. This requires an explicit definition of what information is required before any analysis can proceed. At the conceptual level it is common not to know every piece of design data but estimates can be made and updated as the process continues to develop. This requires a system that can not only handle all the data, but allows these updates to be made, records them and remembers any results associated with them.

The second method utilises information management systems which records the design process data and changes to the data set. They enable design teams to share information and maintain a record of how designs have been created. A management system contains the information which describes a process and has an interface which allows for additional methods to be added on. It is expected that accessing a database through a management system will result in a longer evaluation time than would occur if an object oriented analysis tool was developed.

3.1 The Management System

An information management system must contain data relating to the area of interest of design. The system must be easily extensible, reuses data where possible, can be attached to other design packages, and is accessible by interested parties. The system must also be consistent with the design procedures used later on in the design process and it must be able to reference design databases. Three systems lend themselves as being suitable to be used, n-Dim [19], Épée [20] and a WWW management system [21].

Robertson et al [19] have produced the n-Dim system. The n-Dim package controls access to the database and provides a method of linking between different objects. Links are labelled and the relationship between objects can be viewed. The main advantage of the n-Dim system is that it is fast, maintains object history and has access management facilities. Models can be entered into the system using the ASCEND (McKelvey et al. [22]) equation-based modelling environment. Design packages exist but unfortunately very few process system design tools are written in the ASCEND language. It is not proposed to change the tools used in design and therefore the n-Dim system fails to meet with the requirement to be consistent with the design procedure.

The épée system (Ballinger at al. [20]) provides interfaces to a set of standard, but extensible process engineering objects. The main advantage of the épée system is in providing interfaces to a wide range of applications and enabling them to communicate with each other. The system is also inherently distributed allowing group work to be carried out and records the user's activities for auditing purposes. Épée would appear to satisfy all of the requirements for a suitable management system, however it is cumbersome and requires significant development and support for the client-server architecture.

Andrews and Ponton [21] have developed a World Wide Web (WWW) management system. It exploits the standard client server architecture and enables access to anybody with a web browser. The system interfaces to a wide range of design tools and has access to any database linked to the WWW, also included is an auditing tool which enables reuse of data. The method involves storing information as a collection of HTML documents. Links are created using hyperlinks and can connect to non-HTML files. The system is not as strict as n-Dim in limiting access and potential mutilation of data. However, it does provide a very flexible system and allows the user to add a wide range of development tools.

The WWW management system satisfies all of the criteria for a suitable system and is the chosen method utilised for the development of post synthesis analysis.

3.2 Interface to Post-Synthesis Analysis

A process can be broken down into stream and units, with a topology holding the process together. The WWW management system stores each of these divisions as objects in the format of an HTML document with data about the object being stored in data slots. For example `streams`[1] have compulsory slots which contain flows of each chemical species, temperature, pressure and the phase. The user also has the ability to add any further information slots to the object as required. Analysis methods can be applied to these objects for example to examine the history of creation of an object. `Topologies` which describe the relationship between streams and units can also generate spreadsheet, Aspen and Hysys models of each process.

It is intended that synthesis will be carried out using the CHiPS[2] [23] package to generate a set of alternative solutions to the design problem. The management system is flexible enough to allow for a pre-synthesis stage to be carried out. To perform synthesis the information required is the available feed streams that the synthesis package can use, along with the technologies that are available, and acceptable products that the synthesis stage can produce. The information about the technologies available can be stored in `units`. The search procedure can be modified by also including an `initialisation object`, which states the ability of the synthesis package to use recycles or more pressure states. These objects combine together to form a `task` which can not only generate the synthesis input file, but also a spreadsheet with all of the component information present. The `initialisation` object has a similar format to a `unit` object. The `task` object keeps all of the task information together has a similar structure to a `topology`. Because of this similarity methods which can be applied to a `topology` object such as the generation of a spreadsheet can also be applied to the `task` object.

The solutions generated are placed in the `domain` of solutions, which is in turn split into two different sections, feasible and infeasible solutions. Initially all processes that

---

[1] WWW objects are referred to in `typewriter font`

[2] The system is not limited to the the use of the CHiPS package, any synthesis method can be employed including manual generation

are generated are considered to be feasible, but upon closer inspection some may have undesirable features that would make them prohibitively difficult or expensive to implement. To record the existence of these processes and to ensure re-use of information the infeasible division of the domain has been included. The objects of processes which fall into this division are compressed and are not available for analysis.

Within the domain of feasible solutions there are subsets of processes which share common features such as those processes generated using the same synthesis run or those that satisfy a particular goal. These processes are contained in a `class` as a subset to the **`domain`**. Any synthesis run should generate a new `class` and place the generated processes within it. Both the **`domain`** and the `class` only contain **`topologies`**. The user has the option to select a set of processes and move these off into a separate `class`, and it is on the `class` that post synthesis analysis will be carried out.

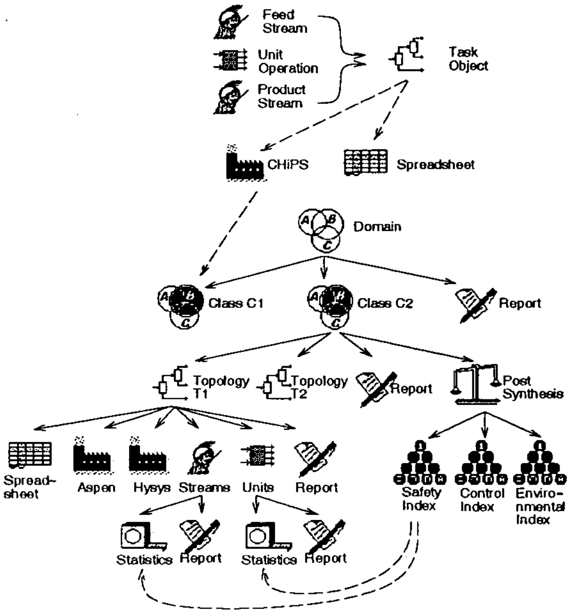


Figure 3.1: Synthesis Environment

Figure 3.1 shows how these objects link together where a solid line shows hyperlinks which are contained within each object and the dotted line links of generated information from an object. These objects do not define all the information which is required before post synthesis analysis can be carried out. For example the environmental view of a waste stream depends upon if the stream is to be released into the environment or sent for further processing. Therefore streams and units also have `statistics` associated with them which contain this extra data. A separate `statistic` object can be regarded as a database which can be linked to a number of different streams and units saving space and ensuring that the most current information is used. `Statistics` do not necessarily have to be associated with a particular object, instead they can reside anywhere upon the web and be linked to by any other object. Therefore a database can be created and maintained across the whole design team to utilise the most current information. `Statistics` are self appending objects meaning that only one copy of the file is created and additional information is added on. Previous values are kept within the file, removing the need for a history file. All the other objects described so far are self replicating objects so that every time the object is updated a new instance of an object is created, and the history log is adjusted.

All of the data required for post synthesis analysis is contained in the `class`. Safety analysis, Control analysis etc. can be applied to each `topology` and a report generated. The results are linked to a `report` which attaches to each `stream` and `unit` in the `topology`. `Reports` also record which statistic values have been used in the analysis giving an auditing trail as to how the result was generated.

The user therefore has the ability to develop a number of different designs and assess their potential impact. Streams and units used in the synthesis stage are consistent with those developed and therefore a cyclic approach to design can be taken and downstream synthesis can also be carried out on these objects.

As the design progresses extra reports will be generated, hyperlinks can be attached to these reports and to relevant objects in the management system. This then gives a system which can be used through the whole process of design.

Chapter 4

Post Process Synthesis Methods

The aim of post synthesis methods is to help the engineer to answer the question 'Which design is best?'. All post synthesis methods require a process structure which is capable of achieving a specified goal. Post process synthesis methods allow for assessment of the process, identification of problems with the design and recommendation of improvements to be made. They are useful tools capable of probing the depth of design without using detailed design information. Assessment methods exist which are capable of examining one issue at a time. This thesis aims to bring together a number of assessment tools which are reviewed in this chapter along with examples of their applicability to conceptual design.

The most utilised method is cost, where a process is designed so as to a achieve a minimum cost requirement. However the cheapest process may not be chosen due to the associated risks caused by the financial markets. Also, if the chosen design fails to satisfy all of the chosen criteria then extra equipment has to be added on to the process. Therefore to base a value judgement upon one indicator would be foolhardy.

Assessment methods can be broken down into two sections either indexing methods or methods that interface for further design. Indexing methods are capable of returning a quantitative assessment of the process and can rank the design of one process against another. An interface for further analysis relies upon methods that give a qualitative assessment of each process, they are incapable of ranking the design and require input from the designer.

Methods to assess the safety of a process, the environmental impact, controllability and flexibility exist. Most require a detailed design in order to give truly meaningful results, but many design features are inherent at the conceptual level and searching this space can give an early insight into the problem. This is done using a short cut analysis tool for each criteria applicable at the conceptual level.

Ideally each method should be similar to the methods used at a detailed design stage so that layers of design can be added on and should an error within the analysis occur, it can be tracked back and corrected at the conceptual stage.

4.1 Costing Measures

The aim of process synthesis is to develop a process which creates new material wealth. Cost has always been of critical importance in the evaluation of conceptual process plant designs as the main measure of material wealth and is fundamental at each stage of design. Design is a creative process and usually goes through a number of distinct stages described by Peters [24] which can be broken down into feasibility study, process design development, general design, accurate cost estimation and optimal design. Cost estimation tries to get close to the actual cost that will be experienced in the future and once complete is substituted by accounting which tells us the exact historical cost, and forecasting which predicts market forces.

Feasibility study

A feasibility study assesses if a process is capable of making money just on the input-output structure utilising available chemistry. The feasibility study is concerned with the environment into which the process is to be placed such that market forces need to be examined to assess if a suitable sized market exists for the volume of product to be produced and if the product specification is suitable.

Process Design Development

Process design development involves developing the basic idea encompassing data and process information. It is at this stage that synthesis techniques to generate conceptual designs are employed. Capital cost estimates are developed along with probable returns. This is the point where a determination about providing capital for the venture can be made.

General Design

General design adds more detail into the design including plant layout, materials of construction, structural design etc. Cost estimates can then be made of all the pieces of equipment and resources that need to be allocated to the project. Cost estimation programs exist such as the Aspen [25] costing package to help evaluate the cost, which includes more detailed calculations for labour costs, site preparation, piping costs etc.

Accurate Cost Estimation

Once a general design of the process is achieved with the size and material of construction of each process unit known actual cost of construction can be evaluated. Direct price quotations from contractors can be asked for. At this point a review of the process design development costs can be made.

Optimal Design

Finally a number of design alternatives exist and the most appropriate process which brings the best profit should be chosen. Optimal design takes all of the information available and examines the sensitivity of the profit of the process to external forces. Also examined is the possibility of cost savings through production techniques, this is the start of an ongoing process of optimisation during the lifetime of the plant to extract most value.

4.1.1 Conceptual Design

Conceptual design fits into the process design development stage where an outline of the design exists. Assessment of each design early on allows for fewer designs to be designed in detail and hence ease the optimal design considerations. Cost estimation not only establishes the viability of a project but is also essential to overall planning. It provides information about the magnitude of the investment and forms the basis for cost control of the project.

It is important to have costing measures which are as accurate as possible, and consistent so that alternatives can be compared on the same basis. Where a product is made on a regular basis good historical data can be used. However, for the chemical industry, which frequently has to make a one off process, accurate estimation of each piece of process equipment is required. Guthrie [26] brought together these two objectives for the purpose of capital cost estimation. The cost of units is based upon 1969 prices for carbon steel pieces of equipment. Many synthesis techniques use the cost correlations developed by Guthrie and update them to modern prices using a Marshall and Swift index. Douglas [3] utilises this method of costing in the hierarchical design method.

Synthesis tends to focus upon the capital cost of the project, selecting those processes with lowest expenditure. Startup and commissioning costs tend to be evaluated using rules of thumb such as Lang factors which estimate the installed cost from the delivered equipment cost.

However, these estimation factors are very basic and fail to meet the criteria set early on in being able to be carried forward for further design. Any revisions to the factors are difficult to re-implement back into synthesis. As one stage of design is complete a new set of costing is created, and therefore a method of recording the costing method and result data throughout the design is desirable.

4.1.2 Post Synthesis Cost Environment

The cost structure for the design of each unit in the synthesis stages is stored in a Web object similar to a `unit` object. Because the results obtained from the synthesis stage also have a link back to the `task` object, the costing used for each structure can be found. The user can then use the synthesis costing equations or apply their own costing measures. This means that costing calculations which are suitable for synthesis can be replaced with more detailed calculations.

The most common form of analysis of cost is through a spreadsheet package, as it gives transparency of all the figures, therefore the post process package returns a spreadsheet file which can be examined by the engineer. This gives the engineer greater flexibility to assess the plants costing over a variety of different conditions and graphs of relevant data can be plotted.

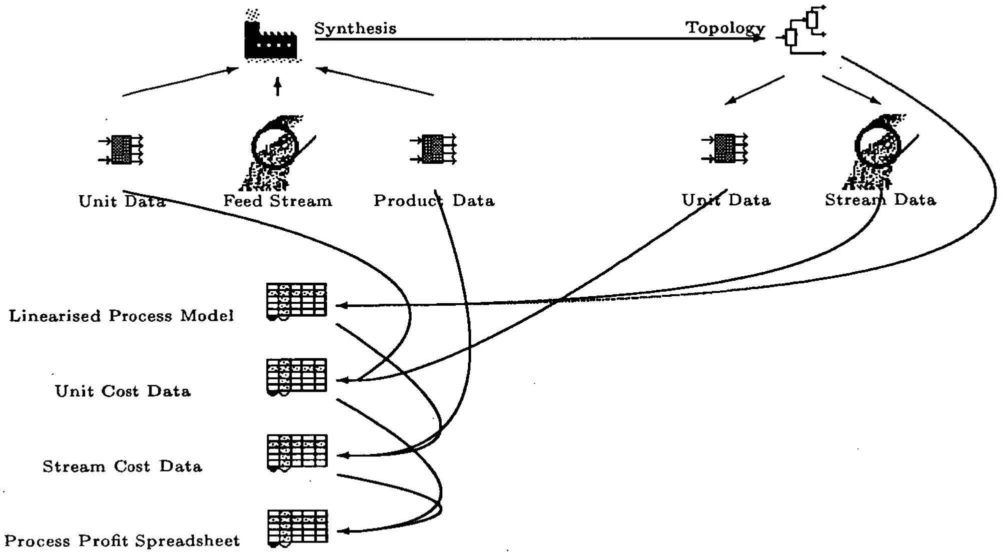


Figure 4.1: Formation of the Cost Spreadsheets

Figure 4.1 shows how the spreadsheet model is formulated in four parts from the synthesis data. A linearised process model of the process is created from the `stream` data and the `topology` of the system. This allows the user to assess changes in the flow and recovery of components.

Data about the size, pressure and temperature of operation are extracted from the result files, along with data about any other pieces of equipment which have been sized during synthesis. All of this information is then collected into a unit cost data spreadsheet which allows the user to revise any capital costing variable.

Synthesis has been carried out knowing the desired products and their respective cost. This information is collected along with the actual product streams. The specification placed upon each product stream is used along with the stream flows generated by the linearised model.

The two spreadsheets relating capital cost and operating cost can then be combined to form a process profit spreadsheet which gives a summary of all cost throughout the plant and allows for present value analysis to be performed. Also included is the ability to assess the plans net present value NPV, internal rate of return IRR, along with other accounting measures. Therefore, the revised costing can contribute to formulating a profitability risk assessment.

4.1.3 Costing Methods

Interpretation of the data contained in the spreadsheet is important as economic measures are the key measure for making project decisions. Assessment of the profitability of the process is dependent upon the cost analysis method used. There are basically two different approaches that can be used depending upon if they discount to present day prices. A review of these costing methods applied to chemical plant design is given by Baasel [27], Peters and Timmerhaus [24] and Chauvel et al [28].

Direct Costing

Direct costing is the simplest method of costing for a process and is the method employed by the CHiPS package for synthesis. A total capital cost for units is evaluated along with the value of streams. Providing that the lifetime of the plant is known then a simple summation can be carried out.

$$Total\ Cost\ = Capital\ Cost - \sum_{1}^{n}(Sales\ Revenue\ -\ Production\ Costs) \tag{4.1}$$

However total cost can obscure information about the actual profitability associated with each design. Consider the following system where two processes can be purchased,

Year	0	1	2	3
Process 1	-10	6	6	6
Process 2	-20	10	10	10

process 1 can be purchased for $ 10 producing returns of $ 6 per year or, a larger process 2 can be purchased for $ 20 giving returns of $ 10 per year.

The profit from process 1 is $ 8 and for process 2 is $ 10 therefore selecting process 2 results in a higher profit. However this analysis does not reflect the true cost of investment. Doubling the investment in process 1 increases the overall profit to $ 16. A useful indicator which normalises the investment is to use payback time.

$$Payback\ (years) = \frac{Total\ Capital\ Cost}{Yearly\ Sales\ Revenue\ -\ Yearly\ Production\ Costs} \tag{4.2}$$

This also has the added advantage in that it is used as a rough measure of risk. A shorter time to re-coup investment means that the process is exposed to a smaller risk.

Discounted Costing

Direct costing does not reflect the true economic conditions that a process will have to operate in. Market pressure demands that an interest rates need to be considered when evaluating the cost of a project. Discounting cash flows so that short term returns are favoured results in two methods that are suitable for cost estimation. The first method is net present value (NPV) which assess the value of a process given the interest rate, capital investment and probable returns over the lifetime of a process.

$$NPV = Capital\ Cost + (Sales\ Revenue - Production\ Cost) * \sum_{i=1}^{n}(1 - \frac{r}{100})^i \tag{4.3}$$

n = Plant lifetime (years)

r = Interest Rate (%)

The second method is internal rate of return (IRR) which assesses the interest rate at which the process fails to make a profit and is evaluated by setting the IRR equal to zero.

These measures are much more reflective of a real scenario, but it can obscure some of the information. NPV is dependent upon the interest rate chosen and IRR does not show anything about the scale of investment.

It is important to assess all costing measures together to gain an accurate picture of the process.

4.1.4 Uncertainty in Costing

In order to achieve an accurate model of cost estimation it is essential to understand the uncertainty associated with the design. Sweeting [29] has shown how to apply statistical methods to determine the spread of operating data and hence the risk associated with each design.

For example, when assessing the design economics during the synthesis stage it makes sense to take the mean value for feed stocks and products over the past few years[1]. This mean value gives an estimate as to the economic operating conditions the process is designed for and is the easiest measure to work with especially if the deviation is assumed to be symmetrical. A median and mode measure can also be employed to assess the centre of deviation and in some cases may be appropriate, e.g. mole fractions where the concentration is frequently 0.99 but can fall as low as 0.97 but is impossible to exceed 1.

Using the centre of distribution is only truly useful when combined with a measure of the dispersion of distribution. If the mean value is used then the dispersion can be

---

[1] Taking inflation into account and discounting accordingly

evaluated as the variance of the system.

$$variance = \int_{-\infty}^{+\infty} (x-\mu)^2 f(x) d(x) \tag{4.4}$$

μ = Mean Value

A more useful approach is to refer to the standard deviation σ which is the square root of the variance and is measured in the same units as the mean. Therefore the standard deviation and the variance are amenable to mathematical manipulation.

One of the main interesting points is the confidence interval so the range of distribution can be seen. The selection of the confidence interval is a user choice but commonly a 95 % value is chosen. For any point on the distribution curve the Z value can be evaluated if the mean and standard deviation are known.

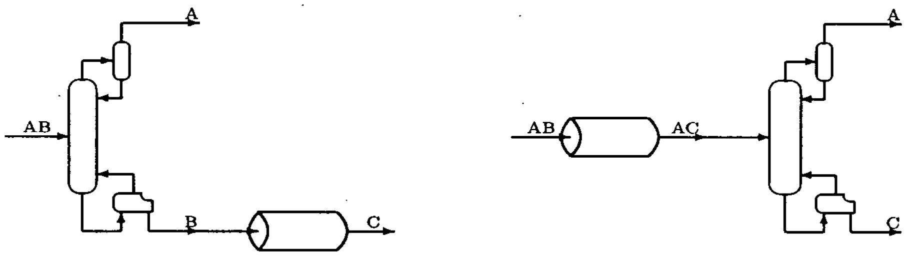
$$Z = \frac{(x-\mu)}{\sigma} \tag{4.5}$$

therefore for a 95 % confidence interval the two points are given by

$$\begin{gathered} P[-1.96 \leq z \leq 1.96] = 0.95 \\ x_1 = \mu - 1.96 * \sigma \\ x_2 = \mu + 1.96 * \sigma \end{gathered} \tag{4.6}$$

4.1.5 Costing Development Case Study

In order to show the differences between the costing measures a case study has been developed using two processes with different capital and operating costs. Synthesis has been carried out in order to produce two components A and C from an eqimolar stream of A and B. The study considers two process units which either separate a process stream using a distillation column or use a reactor to convert B into C. The capital and operating cost of each unit is dependent upon its size. Using this information, process synthesis has been carried out resulting in two viable structures shown in figure 4.2 with the process economics shown in table 4.1.



Process 1

Process 2

Figure 4.2: Development Cost Case Study Topology

	Capital Cost ($)	Operating Revenue Per Year ($)
Process 1	110,000	25,000
Process 2	85,000	21,000

Table 4.1: Process Case Study Economics

Process 1 requires a higher capital outlay for construction, but returns a higher operating revenue than process 2. Using a simple direct costing method with an expected lifetime of ten years the synthesis stage returns an overall profit for the system at $\$140,000$ and $\$125,000$ for processes 1 and 2 respectively. This makes process 1 12 % more profitable than process 2. The disadvantage of this method is that the true value of each process at varying interest rates is not shown. As the interest rate is increased it becomes less advantageous to invest in high capital expenditure projects.

Applying discounted costing enables the desiger to calculate the expected profit at varying interest rates. Figure 4.3 shows the profitability of both processes at interest rates from 0 % to 30 % . It is noticeable that as the interest rate is increased the NPV for process 1 decreases at a greater rate than process 2 until a crossover point is achieved at 9 %. If we consider that 10 % is a useful evaluation point for assessing

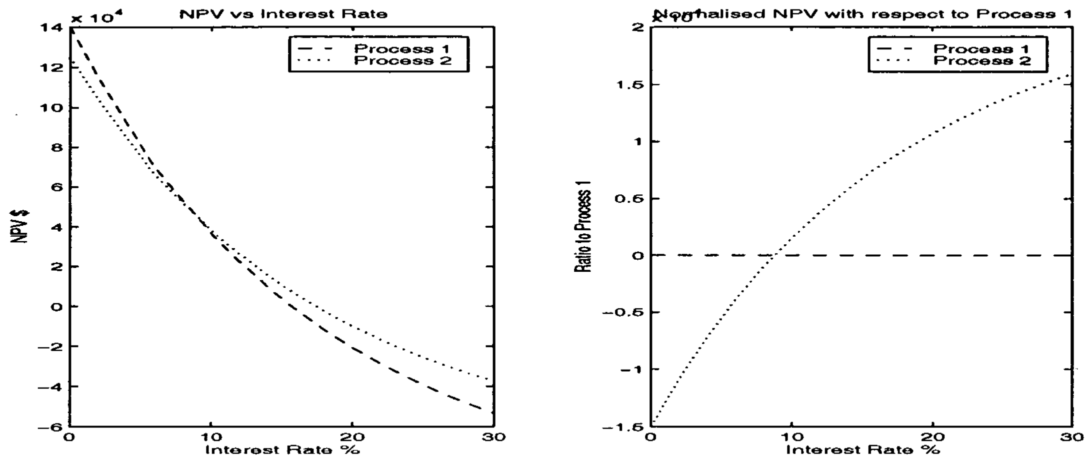
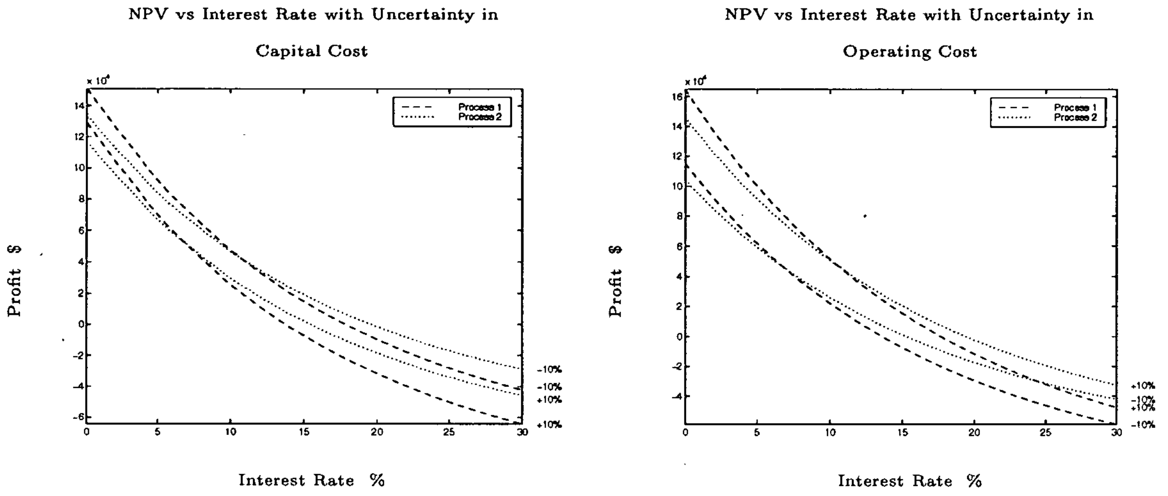


Figure 4.3: Process Cost vs Interest Rate

the viability of production then the two processes are too close together to differentiate upon the basis of cost alone.

The internal rate of return upon for each process shows the interest rate that can be tolerated by each system before zero profit is obtained. For process 1 the IRR is 15.7 % and for process 2 the IRR is 17.4 % . Pay-back indicators show that both processes have a similar pay-back time of 4.4 and 4.0 years for process 1 and 2 respectively. This shows that process 2 is less sensitive to changes in the economic climate and is the process that is exposed to less risk.

Economic factors are not limited to the interest rate, but also uncertainty in the selling price and capital cost of the project. If enough processes are designed and developed then the standard deviation expected for capital and operating cost can be estimated accurately. For an initial estimate a standard deviation of 5 % for the capital and operating cost can be used. Therefore examining a ±10 change in the cost and profit gives the 95 % confidence interval. The boundaries for the economic profitability can be evaluated, and is shown in figure 4.4. Along with the boundaries the graphs also show the interest rate at the point where the process fails to make a profit. This all helps to demonstrate the risk associated with the design. From this analysis it can be seen that process 1 has a higher risk associated with it, and it does not pay back the potential returns in the future when compared to process 2. So where the synthesis stage indicates that 12 % increase in profit could be achieved through the selection of process 1 over process 2, this level of return would not be seen in an economic environment. At higher interest rates of about 15 % process 1 is likely to fail to make a profit and the risk associated with the design does not compensate for the higher investment required when compared to process 2.


NPV vs Interest Rate with Uncertainty in Capital Cost

NPV vs Interest Rate with Uncertainty in Operating Cost

Figure 4.4: Process Costing with Uncertainty Conditions

Each spreadsheet model incorporates a linear model of the process system so perturbations to the operating conditions can be made. Changes to the feed stock, reactor conversion or distillation recoveries can be made. The two processes presented produce similar results to any disturbance placed upon them. Therefore a better measure of their effectiveness to deal with changing conditions is to examine the effect of uncertainty in the operating conditions.

4.2 Safety

Safety or hazard analysis and risk assessment has always been a critical feature of any chemical plant design. As a process is developed many reviews of the safety of the process will be carried out. The aim of safety analysis is to determine if a combination of events can lead to an unsafe situation. Lees [30] states that 'The safety of a plant is determined primarily by the quality of the basic design.'. We are helped by the fact that at the conceptual level of design, there is the strong potential to eliminate hazards rather than devise methods of control. Lees [30] shows some of the design principles which have to be considered in order to achieve a suitably safe process design:

Inherently safe processes. If a process can be designed so as to use less hazardous materials or avoid extreme operating conditions then safety can be built into the fundamental design of the process. The idea being that what is not there can not blow up or leak into the environment (Kletz [31]).

Limitation of Inventory. By avoiding holding large inventories of hazardous material, the riskiness of the design can be reduced.

Process Operability. Some processes are more operable than others. Systems which have a number of safe states of operation that the operators can resort to in case of emergency can be considered to be safer than those processes which require an immediate and total shutdown.

Fail Safe Design. Processes should be designed so as to select equipment that can operate safely due to unforeseen circumstances such as a utility failure.

Second Chance Design. Accepting that failure will occur, processes that have the ability to protect against further damage can be considered safer.

System Size. Large complicated systems tend to be less manageable, require complicated control structures, require more operator training and hence they are more prone to error.

The most appropriate method for safety analysis depends upon the system being analysed. Guidelines exist [32] to help determine the most appropriate method with most working around the idea of identifying an incident scenario leading to a possible accident, and assessing the possibility and consequence of the event occurring. This should therefore give an index of risk which can be used to optimally design the process and provide an acceptable risk. The most difficult part of which is identifying potentially hazardous events. Kletz [33] shows how a Hazop study which is a systematic search for hazards can be employed to help the designer find potential hazards.

For conceptual design Wells [34] shows that the best method to start a new hazard study is to identify the main hazards and hazardous conditions with Concept Hazard Analysis. It is similar in implementation to a Hazop study but tackles the problem by assuming that an incident will occur. It is intended to work with a committee and splits the problem down into manageable sections focusing upon major hazards. However, Concept Hazard Analysis is poor for identifying the root causes of incidents and checking the control systems that would have to be put in place. The assessment method applied to conceptual design can only make an estimate of the risk and the potential damage. None the less it is a very good analysis to identify the major hazards and can help to identify if the management and local environment can cope with the impact of the project.

Concept Hazard Analysis is the first stage in safety analysis and if managed correctly should be similar to a Hazop study which is the main focus of a safety review. A Hazop study is primarily aimed at detailed design once again breaking the process down into manageable sections. Hazop studies rely upon identifying causes of safety problems and when combined with a fault tree analysis and task analysis gives the ability to formulate a complete risk assessment. Fault tree analysis is widely used to demonstrate system failures and can be used to quantify the probability of frequency of failure. Task analysis takes a task objective and breaks it down into sections. It is useful in assessing an operation and is commonly used when the state of a process is changing. Task analysis is useful for writing operating procedures and understanding the general nature of an operating problem.

Hazop does not identify how things could of been done better and inherent safety is best identified through Critical Examination. Critical Examination is described by Wells [34] as a self reflecting process where the design team finds out if this was the best way to design a process. It is best handled at the conceptual level but can reappraise the fundamentals of any process. The relies upon creative thought to reduce the hazard by examining if things can be carried out better. Each of the methods enable the design team to identify potential hazards, with each method giving different recommendations for hazard control.

4.2.1 Hazop

Hazop [35] has become one of the standard tools used to assess the safety of a plant and examples of implementation are given by Kletz [33]. A Hazop study is a systematic examination of how process deviations can propagate as hazards. In many cases it has become mandatory because of its proved capabilities. While it is difficult to apply at the conceptual level it will be one of the main points of any safety analysis. Conceptual design analysis should be consistent with it so assumptions that are made early on in the design can be checked and re-evaluated if necessary.

The main benefit of a Hazop study is that it can recommend improvements to the design. It can be applied to both a new or an existing plant and the recommendations tailored respectively. In most situations Hazop is an ongoing procedure and reviews will have to be carried out through out the life time of the plant.

In order to perform a full Hazop study a P&ID is required of a detailed design. Hazop also requires identification of significant deviations that can occur and normally the judgement and experience of people closely related to the plant needs to be utilised. Hazop is carried out as a team activity ideally utilising a broad range of skills and knowledge of past events.

A Hazop study first selects a process deviation, identifies if this is a hazard and then considers changes that would lead to an improvement. The study is then carried out for all deviations to the system. Computer support for the hazard analysis has been developed by Bunn and Lees [36] and Waters and Ponton [37] [38] which tackle the problem by developing expert systems to assess process designs.

At the conceptual level Hazop is not entirely feasible to implement as there is insufficient information from the process flowsheet and the user has a limited amount of input into the system. The main problem with a Hazop study is that it is tedious and time consuming, which is a problem when considering a number of flowsheets. At the conceptual stage it has also been found that Hazop study has not proved satisfactory as it has inhibited creative thought in the design of alternative methods of production with recommendations that tend to supplement the original design.

4.2.2 Concept Hazard Analysis

Concept Hazard Analysis described by Wells [34] is used for the identification of hazard characteristics in an attempt to identify areas which are particularly dangerous. The main advantage of Concept Hazard Analysis is that it can be commenced at a point when the preliminary process flow diagram is available and is aimed at identifying hazards and any preventative measures that may need to be taken.

At the conceptual stage of design the problem is how to identify each of the potential hazards. A similar study to the Hazop study developing keywords and then identify the methods of analysis. For example, using the keyword FLAMMABLES a search is performed through the process and identify all sources of flammable release, assess if the release is dangerous and propose reduction measures.

One method of reducing process hazards is by Critical Examination which examines if we really have to produce using this method, and instead searches for better and less dangerous ways to carry out a process. Therefore processes which are easier to control, or have less dangerous material within them are considered to be inherently safer plants. Concept Hazard Analysis is focused upon the consequence of an event and not upon the frequency of the event.

In order to calculate the hazard risk from Concept Hazard Analysis requires calculating the hazard of each keyword.

4.2.3 Indexing Methods

Indexing methods of safety are specific to certain keywords in the hazard analysis. They can help to identify possible event scenarios. Because they focus upon a specific problem they cannot cover every possible event. The user must be careful not to be given the impression of a safe process due to a set of low index results. The indexing methods have been devised for a specific situation and may not be applicable to the situation being considered.

4.2.4 Fire and Explosion Index

The most common indexing method used in safety analysis is the Dow Fire and Explosion Index [39] which has been developed from the Mond index [40]. It is a useful index for determining the relative degree of hazard of flammable and explosive mixtures. The procedure is capable of returning a cost amount for the maximum probable damage. It is useful in assessing the extent of exposure to risk and combined with a risk analysis can form part of a safety appraisal.

The method works by applying penalties for the presence of hazardous items such as flammable inventory, high pressures etc. Credits can be added for having items which increase the safety of a process such as fire protection, emergency power, interlocks etc. At the conceptual level the analysis can be on the core process without any safety features present. This should then help identify any inherent safety features contained within the design and enables comparison between design alternatives. The index examines a particular area of the process which could be the entire process or a particular unit. At the conceptual level the analysis is performed on each `unit` of the process.

The first stage in the analysis is to evaluate a material factor which is a measure of the potential energy release from fire or explosion. It is dependent upon the reactivity and flammability of the components present for which a database is given in the guide. These factors are contained in the component `statistic` object. As the analysis is carried out around each `unit` the `stream` which connects to the `unit` with the highest material factor is used in the analysis. The more flammable the stream the higher the material factor used. Figure 4.5 shows how all of the information is linked together.

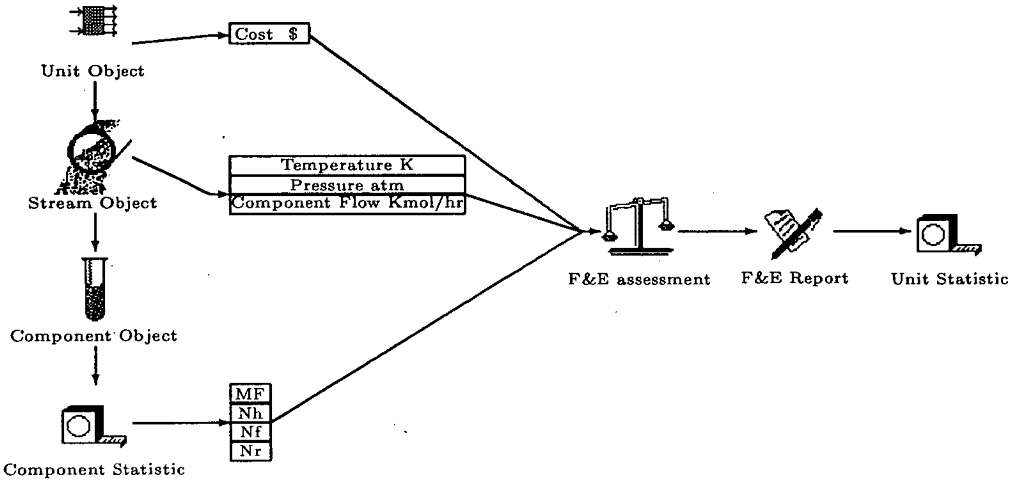


Figure 4.5: Formation of the Fire and Explosion Index

The evaluation is carried out by first evaluating a material factor for each stream. The stream with the highest material factor is then used in the analysis. Also obtained from the stream object is the maximum and minimum temperature and pressure of the streams connecting to the process unit. General process hazards then need to be evaluated which determine the magnitude of loss of an incident. Penalties are accumulated for general process hazards for exothermic chemical reactions, enclosed units, poor access and drainage. Because most of this information is added at detailed design it is assumed that a base factor of 1 will be used which can be increased up to 2.25 if a chemical reaction takes place.

Of greater interest is the special hazard factor. These are factors which contribute to the probability of a loss incident. The twelve factors which can be major causes of fire and explosion are described in the fire and explosion guide [39] and a summary of their respective penalty contributions are shown in appendix B.1.

Once the special hazard factor has been calculated a process hazard factor can be calculated.

$$Process\ Hazard\ Factor = General\ Hazard\ Factor * Special\ Hazard\ Factor \quad (4.7)$$

Multiplying the process hazard factor by the material factor for the unit gives the fire and explosion index. The higher the index the greater the risk and an index of less than 60 indicates a light degree of hazard through to 160 and above which would be indication of a severe hazard.

$$FEI = Hazard\ Factor * Material\ Factor \quad (4.8)$$

The fire and explosion index calculated can be turned into a radius of exposure by multiplying by a factor of 0.256. The radius of exposure is considered from the outside surface of the vessel and therefore the radius of the unit is included.

$$Radius\ of\ Exposure(m) = 0.256 * FEI * Unit\ Footprint\ Radius \quad (4.9)$$

The replacement value of the piece of equipment can be important in assessing the insurance cost of the process. A factor of 0.82 is used to allow for items of cost not lost such as road, foundations etc. An initial failure can create a chain effect of failures to occur and an estimate of the potential to loose more units is possible. This is simplified with an escalation factor for which an estimate of 1.2 can be used for conceptual design purposes.

$$Replacement\ Value = 0.82 * Unit\ Cost * EscalationFactor \quad (4.10)$$

A damage factor which represents the effect of fire and blast damage can be determined from the FEI and the material factor. The damage factor is calculated using equation

4.11 where the coefficients are dependent upon the material factor and given in appendix B.2. The maximum damage factor is 1 and represents units handling highly explosive or flammable materials.

$$Damage\ Factor \ = \ Dfa + Dfb * FEI + Dfc * FEI^2 + Dfd * FEI^3 \tag{4.11}$$

Within the area of exposure it is useful to obtain an appropriate dollar value for the plant equipment which would be lost. This is calculated as the base damage factor and is given in equation 4.12.

$$Base\ Damage\ Factor \ = \ Damage\ Factor \ * \ Replacement\ Value \tag{4.12}$$

Measure which attempt to prevent loss from occurring can be factored into the analysis with a loss control credit factor. Because ancillary equipment which reduces risk is added on at the detailed design stage an estimate of 0.75 for the loss control credit is used.

The actual damage factor represents the damage cost which would be incurred if an major incident was to happen. It is calculated as the product of the base damage and the loss credit factor. The actual damage factor would approach the base damage factor if loss prevention measures fail.

$$Actual\ Damage\ Factor \ = \ Base\ Damage \ * \ Loss\ Credit\ Factor \tag{4.13}$$

Another useful equation is the number of days that the system would be down for in the case of a loss incident. This enables the potential business interruption to be calculated whose cost of which can exceed that of the property damage. An estimate of the number of days outage can be made using equation 4.14.

$$Days\ Outage \ = \ exp(1.32 + 0.59 * log(Actual\ Damage/1000000)) \tag{4.14}$$

For conceptual analysis this is as far as the analysis can progress. Further design will analyse the impact of installing preventative measures. Measures which are installed which add to the process control, material isolation and fire protection can each reduce the fire and explosion index and contribute to the loss control credit factor making the process safer.

The system developed can analyses the process unit by unit. The user can view an index for the whole plant, along with the Damage Factor and the Actual Maximum Damage that would be caused by the event occurring.

4.2.5 Chemical Exposure Index

Facilities which store or handle toxic materials may require an evaluation as to their potential chemical exposure hazard. The Dow chemical exposure guide [41] provides a method for rating the relative health hazard to people in the local vicinity of a possible chemical release.

The index is aimed at detailed design, but can be applied to conceptual hazard analysis and can highlight important aspects of the design that may have to be taken into account. It is useful in evaluating if it is realistically possible to situate a process at a certain location and the emergency response measures which would have to be put in place.

The first stage in the analysis is for the user to determine possible chemical release incidents. This should be performed at the concept hazard analysis stage to ensure that only feasible scenarios are examined. The chemical exposure index can be applied to scenarios relating to the rupture of any pipe within the process. If it is assumed that any stream can rupture then the analysis can be performed over the entire process and risky streams can be identified.

The evaluation method requires information from the data management system. From the streams information about the temperature, pressure, phase, molar flow of components and the diameter of the pipe is required. The component information has to contain information about the physical property of the components and the toxicity of each component. This information is contained in the component `statistic` object. The values for the toxicity of components are published by the American Industrial Hygiene Association [42] as Emergency Response Planning Guideline figures (ERPG). It is useful to start examining the chemical exposure hazard for the entire process using the ERPG-2 figures for each component, which is defined as 'The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to one hour without developing irreversible or other serious health effects or could impair their ability to take protective action.'. The ERPG-2 figure for streams that contain mixtures of components can be calculated using either a potency-weighted addition of the toxicity of components, or by examining the interactions between components as described by Mumtaz et al. [43]. The diameter of the pipe work is unlikely to have been calculated during the synthesis stage and the user will have to enter the diameter in the stream `statistic` object or calculate it with the pipe sizing method discussed in 4.4. The data required to perform the analysis and the location it is stored in is shown in figure 4.6.

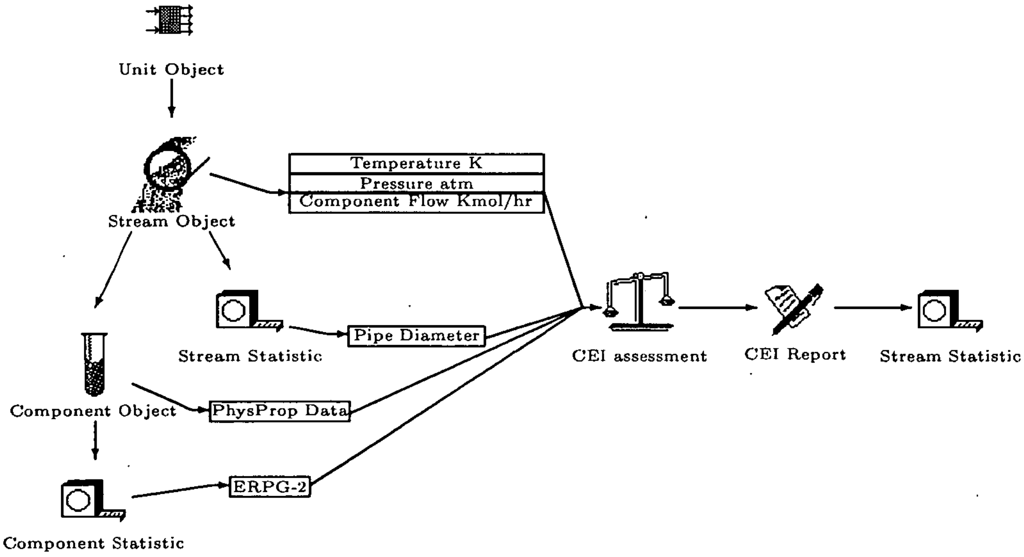


Figure 4.6: Formation of the Chemical Exposure Index

The first stage in the analysis is to determine the amount of material that is released into the atmosphere. If the release is gaseous and the escape release velocity is assumed to be sonic then equation 4.15 [2] can be used to estimate the airborne quantity [41].

$$AQ = 4.751 * D^2 * P * \sqrt{\frac{MW}{T}} \tag{4.15}$$

AQ = Airborne quantity Kg/sec
D = Diameter m
P = Pressure KPa
MW = Molecular Weight
T = Temperature K

Liquid releases require a much more detailed analysis of the airborne quantity released. If the components present in the liquid are non-volatile and released from a low pressure tank then pooling can be expected to occur. However if the converse is true then the release can be expected to flash producing an aerosol effect and carrying small droplets away in the vapour cloud. An intermediate effect can also occur where partial vapourisation occurs producing a pool and a vapour cloud. This means that the system has to have the ability to access a physical property package to evaluate the normal boiling point of mixtures and perform flash calculations.

The first stage in the analysis is to evaluate the amount of liquid which is released. Assuming that the release lasts for at least five minutes then equation 4.16 can be used.

$$L = 0.944 * D^2 * \rho\sqrt{\frac{1000 * P}{\rho} + 9.8 * \Delta h} \tag{4.16}$$

D = Diameter m
L = Liquid Release Kg/sec
P = Pressure kPa
Δh = Height of liquid m
ρ = Density Kg/m^3

The height of the liquid above the release point can be assumed to be 1 metre at the conceptual design stage. The total size of the pool which is formed must then be estimated. The pool is assumed to reach a final size after 15 minutes and therefore the

---

[2] Equations from the chemical exposure index [41]

total amount of material being released is the Liquid release rate times 900.

If the operating temperature is less than the normal boiling point of the liquid then the flash fraction is zero. Otherwise equation 4.17 should be used to determine the airborne quantity caused by the flash.

$$AQ_f = 5 * \left(\frac{Cp}{Hv}(T_s - T_b)\right) * L \tag{4.17}$$

If $AQ_f > L$ no pool is formed and $AQ_f = L$.

AQ_f = Airborne quantity caused by flash Kg/sec
Cp = Heat capacity of liquid J/Kg/ °C
Hv = Heat of vaporisation of liquid J/Kg
L = Liquid Release Kg/sec
T_b = Normal boiling point of liquid K
T_s = Operating temperature of liquid K

Evaporation of liquid from the pool needs to be estimated. The pool size can then be calculated from the remaining material that has not been flashed. The size of the pool can be calculated by approximating the pool depth to be 1cm. If the liquid is below its normal boiling point and above ambient temperature then the pool temperature is assumed to remain at the operating temperature, otherwise the pool temperature is the boiling point of the liquid. The airborne quantity caused by evaporation can then be calculated using equation 4.18.

$$AQ_p = 9.0 * 10^6 * \left(\frac{Wp}{\rho}\right)^{0.95} * \frac{MW * P_v}{T} \tag{4.18}$$

AQ_p = Airborne quantity from pool. Kg/sec
P_v = Vapour pressure of the pool. kPa
T = Pool temperature K
MW = Molecular Weight
Wp = Total liquid in pool Kg
ρ = Density Kg/m^3

The total airborne quantity is the summation of the flash quantity and the evaporation quantity. Once the airborne quantity is known then the chemical exposure index can be evaluated using equation 4.19. The hazard distance in metres is 10 times the CEI up to an upper limit of 10,000 metres.

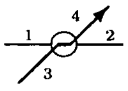
$$CEI = 655.1\sqrt{\frac{AQ}{ERPG-2}} \tag{4.19}$$

4.2.6 Safety Development Study

The development study examines the effect of either 1 large heat exchanger or 2 smaller parallel exchangers with an equal split. Process 1 is shown in figure 4.7 with a capital cost of $ 10,000. The second process is shown in figure 4.8 with a cost of $ 6,000 for each exchanger. Splitting the streams will reduce the inventory of material and reduce the size of the pipes connecting each heat exchanger. Any safety benefit that this gives can be examined and the cost trade off evaluated.

FEI analysis

The system is modelled with web objects and the fire and explosion index applied. For process 2 each mixer and separator is stored as a `unit` object with zero volume and zero cost. The fire and explosion index assesses each of these units and are therefore included in the analysis but they do not contribute to the maximum probable damage caused. The system returns information blind to reality and it is up to the user to overview the results returned from the analysis tool.

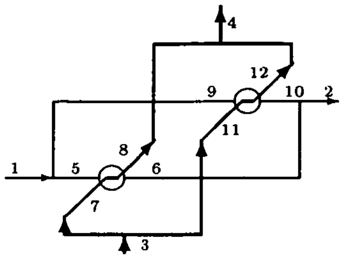


	1	2	3	4
Temp °C	700	60	31	660
Pressure atm	3.3	1.1	2.5	2.3
Flow Kmol/hr	100	100	90	90
Cp KJ/Kmol K	46	46	52	52

Stream	MF	Nh	Nf	Nr	ERPG
1&2	21	1	4	0	900
3&4	24	1	4	2	600

Figure 4.7: Process 1 Development Safety Study

The index is calculated with the results from the mixers and separators removed and



Stream	1	2	3	4	5&9	7&11	6&10	8&12
Temp °C	700	60	31	660	700	60	31	660
Pressure atm	3.3	1.1	2.5	2.3	3.3	1.1	2.5	2.3
Flow Kmol/hr	100	100	90	90	50	50	45	45
Cp KJ/Kmol K	46	46	52	52	46	46	52	52

Stream	MF	Nh	Nf	Nr	ERPG
1,2,5,6,9,10	21	1	4	0	900
3,4,7,8,11,12	24	1	4	2	600

Figure 4.8: Process 2 Development Safety Study

the overall results are shown in table 4.2.

	Process 1	Process 2
FEI	42.96	85.92
Cost $	10000	12000
Damage Factor	1.45	2.90
Maximum Damage $	4 122 000	4 946 000

Table 4.2: Fire and Explosion Results

It would appear from the FEI that process 2 has a much higher index than process 1, but each process is not compared on a similar basis. Process 2 has two units, duplicating the assessment and the hazard associated with it. The only true measure which can be applied on a plant wide basis is the maximum damage and this assumes that every process unit is lost.

The analysis is only truly applicable at the unit level and results from the system relating to the hazard of each unit is returned.

The analysis does not include a risk analysis and therefore we can not say which of the two processes is safer. For process 2 if the two heat exchangers are separated so that the loss of one exchanger does not effect the probability of failure of the second exchanger then the system could be considered to be safer. However, if the converse is true then the system would have an inherently higher maximum damage potential and would be considered to be less safe. The analysis can not show which processes are safe, but can detail the potential possibilities to incorporate inherent safety in the risk analysis.

CEI index

A similar analysis is applied with the chemical exposure index. Before the chemical exposure index can be evaluated more information about the size of the pipes connecting to the units together need to be evaluated. An assessment tool has been included in post-synthesis analysis in section 4.4. For this analysis we will assume a constant pipe size of 5 cm diameter for the hot side stream and 3 cm diameter for the cold side stream.

With the diameter of each connecting pipe known in the stream `statistic` object then the CEI can be evaluated. The chemical exposure for the feed and product streams is shown in table 4.3.

Stream	CEI	Airborne Quantity (Kg/sec)	Hazard Distance (m)
1	62.0	8.05	619.7
2	46.8	4.6	467.7
3	53.0	3.9	530.1
4	38.4	2.1	384.2

Table 4.3: Chemical Exposure Results

Performing an equal split on each split reduces the potential exposure of each stream the results are shown in table 4.4. For each unit particular attention has to be paid to the stream with the highest CEI. The hot side temperature feed stream has the highest CEI and hence the largest hazard distance associated with it.

Using two heat exchangers reduces the hazard distance of each unit down from 620m to 430m. This assumes that the mixing and separating joints are perfect and unlikely to fracture. The overall area exposed is reduced and the two heat exchangers would appear to have more inherent safety. To gain a full understanding of the process a risk

Stream	CEI	Airborne Quantity (Kg/sec)	Hazard Distance (m)
5&9	43.4	3.9	433.8
6&10	19.4	0.5	194.4
7&11	32.7	2.2	327.4
8&12	14.1	0.3	140.9

Table 4.4: Chemical Exposure Results

assessment would have to be carried out to establish the probability of release.

4.3 Environmental Analysis

The move towards providing processes which provide sustainable development places pressure on the designer to choose the best process with the smallest influence upon the environment. Assessment of these issues is a well recognised process during design. Selection of a highly polluting process to produce an 'environmentally-friendly' product (e.g. bio-degradable) would be unsuitable. Therefore, good product policy takes into account the entire life-cycle of a product and returns this information so as to better inform the general public. A life cycle assessment takes into account hidden details about production such as the cost of building the plant and the final disposal of the product. This should lead to better production methods and more environmentally friendly products.

Environmental issues are diverse and frequently an improvement in one area can only be made at the expense of another. Environmental issues such as depletion of abiotic and biotic resources, enhancement of the greenhouse effect, depletion of the ozone layer, human toxicity, ecotoxicity, photochemical oxidant formation, acidification, nutification and odour all need to be assessed before an understanding of the environmental impact can be made. Many environmental methods assess the performance of a process by comparison to acceptable limits. At the conceptual level the desire is to identify the process with the best inherent environmental features.

Steffans et al [18] has incorporated environmental indexing methods into process synthesis, introducing two environmental impact indicators of life cycle analysis and a sustainable process index. Synthesis is carried with an assessment into cost and environmental impact being performed simultaneously along with a multi-objective analysis method. The disadvantage of this method is that it relies upon being able to reduce the problem to a single objective function.

4.3.1 Assessment Methods

Sharratt [44] shows the criteria that a computer aided environmental assessment should satisfy. The main points are that the assessment method should be unbiased so that with perfect input data the method will give the actual environmental impact of the process. The assessment should not ignore any impact from the process for example the effect of accidental releases. The measure should also be meaningful and transparent so that a clear direct environmental impact assessment can be made. Assessment methods which are available to the designer are life cycle assessments, substitution/elimination indices and the sustainable process index.

Life Cycle Assessment

To assess the effect of production of a material from the cradle requires life cycle assessment (Metry [45], Zanetti [46]). For a chemical plant life cycle assessment (LCA) can be regarded as an auditing tool where the boundaries are drawn around the process flowsheet. The environmental impact of everything entering and leaving the system must be accounted for. This includes the process streams, energy consumption, and any environmental influence caused through production. As an indexing method LCA can be used an auditing tool comparing inputs to outputs where a lower figure is more desirable. Negative LCA is possible and does not necessarily mean that the process is the best solution as it has to be compared to other alternatives. LCA can also include the environmental cost of building and maintaining the process. A complete life cycle assessment can be difficult to implement as accounting for the effect of every material present and its effects can be laborious.

Figure 4.9 shows the system boundary for a distillation column. The effect upon the environment of all input and output streams needs to be assessed for an impact study to be performed.

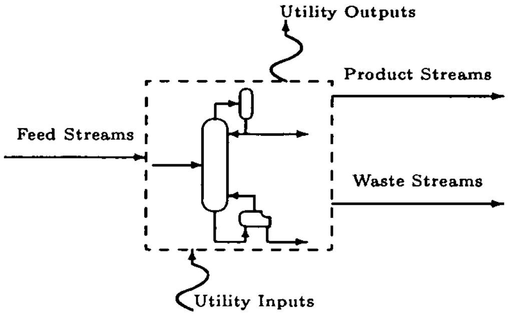


Figure 4.9: System Boundary for a Distillation Column

Substitution/Elimination Index

The substitution/elimination index described by Brennan [47] is a useful tool utilising information from the output of the system boundary. Processes can only be improved by either substituting for a more environmentally friendly substance, turning waste into product or eliminating pollutants from the system. Like the LCA it requires boundaries to be drawn around the process and the impact of all inputs and output to be accounted for.

$$Substitution/Elimination = \frac{Waste\ and\ Product\ Stream\ Impact}{Product\ Stream\ Impact} \qquad (4.20)$$

The substitution/elimination index enables processes of differing scale to be compared and gives an indication as to the room for improvement. The index can also include feed streams as a negative term in both the numerator and denominator and is also applicable to energy assessments. The assessment is easy to implement but care must be taken to ensure that it does not favour the production of environmentally damaging products.

Sustainable Process Index

Krotscheck and Narodoslawsky [48] have produced a measure of the sustainability of a whole process. The idea is that a specific area of land is required in order to sustain a process and a measure of this area gives an indication as to the environmental impact of the process.

4.3.2 Depletion of Abiotic and Biotic Resources

The combination of study into the depletion of abiotic and biotic resources gives the best indication of the environmental impact of a process, but these are difficult to quantify. The depletion of abiotic resources is considered by comparing the quantity of material used against the reserves available.

$$Abiotic\ Depletion = \frac{Material\ Used\ (Kg)}{Reserves\ (Kg)} \tag{4.21}$$

Abiotic depletion is most appropriate for analysis into oil consumption and metal consumption. Where reserves are unknown or unsure or situations where recycling may become more prominent the use of abiotic depletion for planning purposes may lead to misleading action being taken.

Biotic depletion is even harder to quantify an the process plant scale. It is the number of animal species threatened with extinction. If it was possible to quantify the impact on biotic resources of constructing a new plant then an accurate environmental assessment would be formed. It would be very difficult to see the impact of a process plant upon a species on the other side of the globe (e.g. impact upon the black rhino population). Contributions to the greenhouse effect, depletion of the ozone layer and increases in toxicity all contribute. Therefore, it is more practicable to concentrate on these directly influenced factors.

4.3.3 Quantifiable Measures of Pollution

Measures of pollution are very broad and tend only to be applicable once a problem has been identified that adversely effects the quality of life or environment. Also they need to be examined with care where the situation of the process has to be taken into account. For example, a processing plant discharging a saline solution may be acceptable on the coast, but not on a freshwater river. Most measures of pollution involve evaluating the quantity of substance being released and relating it to an equivalent amount of reference material. Heijungs [49] gives a review of some of the quantifiable measures that are available.

Enhancement of the Greenhouse Effect

Some substances when released into the environment contribute to the enhancement of the greenhouse effect. Parameters have been developed for these substances in the form of a global warming potential (GWP) so that a single effect score can be achieved. GWP uses CO_2 [3] as a reference material. The GWP is the extent to which a mass unit of a given substance can absorb infrared radiation compared to a mass unit of CO_2 . The GWP is given in 20, 100 and 500 year life times as components undergo change including the photo-synthesis of CO_2 . Table 4.5 gives an example set of global warming parameters from Heijungs [49].

$$Greenhouse\ Effect\ (Kg) = \sum_i (GWP_i * emission_i\ to\ the\ air\ (Kg)) \tag{4.22}$$

Formula	Substance	GWP_{20}	GWP_{100}	GWP_{500}
CO_2	Carbon Dioxide	1	1	1
CH_4	Methane	35	11	4
CF_2CL_2	CFC-12	7,100	7,100	4,100

Table 4.5: Global Warming Potential Parameters

Depletion of the Ozone Layer

Some substances contribute to the depletion of the ozone layer, for which an ozone depletion potential (ODP) parameter has been developed. Similar to the GWP the ODP is a relative parameter and uses CFC-11 as the reference gas and is measure of the steady state ozone depletion per mass unit of gas emitted to the atmosphere.

$$Ozone\ Depletion\ (Kg) = \sum_i (ODP_i * emission_i\ to\ the\ air\ (Kg)) \tag{4.23}$$

---

[3] CFC-12 is also commonly used as a reference gas, so the term GWP should be used with caution

Human Toxicity

Human toxicity is assessed by emissions on an instant, hourly, daily and yearly basis. Data is collected from toxicology experiments about the maximum daily intake or concentration which is acceptable. Emissions are then corrected depending upon how the release is made so that emissions to the air, water and soil can be combined. This then gives a human toxicological classification factor for the atmosphere (HCA), for water (HCW) and for soil (HCS).

$$\begin{aligned}\text{Human Toxicity (Kg)} = \; & \textstyle\sum_i(HCA_i * \mathit{emission\ to\ the\ air}\ (Kg) \\ & +HCW_i * \mathit{emission\ to\ water}\ (Kg) \\ & +HCS_i * \mathit{emission\ to\ the\ soil}\ (Kg))\end{aligned} \tag{4.24}$$

Ecotoxicity

The ecotoxicity is assessed through the use of maximum tolerable concentrations (MTC). It applies to concentration in the soil and the water and therefore two ecotoxicological classification factors are employed (ECA) for aquatic systems and (ECT) for terrestrial systems. The units of measure for ECA is mg of pollutant per m^3 of water and for ECT is mg of pollutant per Kg of polluted soil.

Photochemical Oxidant Formation

Photochemical ozone creation potential (POCP) is similar to GWP. The POCP is also a relative measure using ethylene as the reference component to allow atmospheric emissions are converted to equivalent ethylene emissions

Acidification, Nutification

The contribution to acidification potential (AP) and nutification potential (NP) can be assessed. For acidification the emissions are converted to equivalent sulfur dioxide emissions. Processes releasing nutification compounds can be compared by converting to equivalent phosphate emissions.

Other Measures

Other measures to evaluate environmental impact can also be included. These could include malodourous air, noise, aquatic heat emissions, radioactive emissions etc. Any system developed for assessing the environmental impact must be able to deal with the need to include user defined measures.

4.3.4 Environmental Indexing Method

An indexing tool has been developed using life cycle analysis, which takes into account the components environmental impact and the method of disposal. Streams are identified either as being a flue, purge, landfill, drain, feed or product stream. Components contain information in their `statistic object` relating to their impact upon the environment depending upon the method of release. For example, methane has two slots relating to the global warming potential 'Green_House' for a direct release into the atmosphere and 'Flue_Green_House' for an oxidised release with values of 1 and 11 respectively. The indexing procedure then identifies the stream destination, its respective components and the impact associated with the method of disposal.

Most indexing methods are auditing tools taking quantity of material and its effect upon the environment into account. Therefore, the method employed is to search through all product and feed streams given by the `topology object` and identify the quantity of components which has an impact upon the environment. The system has to take into account both the inputs and outputs from the system, so that life cycle analysis of the process can be performed. Processes which reduce environmental damage can also be assessed.

Indexing methods to assess the enhancement of the greenhouse effect, depletion of the ozone layer and human toxicity have been implemented. Each index is created by collecting data through web pages, accessing the assessment program through a CGI script and reporting back into a web page.

A second method available to assess environmental impact is to examine the power usage of a process. The power usage corresponds closely to the amount of greenhouse gas emissions released into the atmosphere. This is dependent upon the power source. For example, electricity has a higher greenhouse emission per kilowatt associated with it than steam. The energy requirements of each unit can be recorded in the unit `statistic object`.

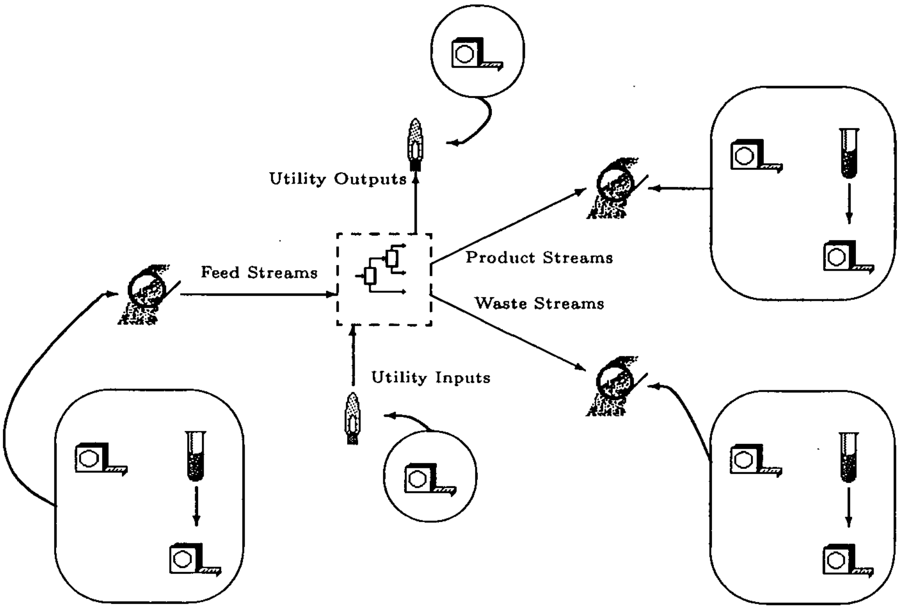


Figure 4.10: Environment Analysis Environment

4.3.5 Environment Development Study

To demonstrate the environmental indexing method a simple case study has been developed. The process oxidises A to B in the presence of oxygen. In order to keep A below the flammable limit and to provide heat for the reaction a methane diluent has to be used. The reaction proceeds so that there is a 40 % conversion of A and 95 % conversion of the oxygen. Product streams that can leave the process are either a flue gas stream consisting mostly of CO_2 , a product stream of B and a sewage stream which is predominantly water.

$$A + O_2 \rightarrow B \tag{4.25}$$

$$CH_4 + O_2 \rightarrow CO_2 + 2H_2O \tag{4.26}$$

Synthesis is carried out and the two structures are shown in figure 4.11 and 4.12 are viable. The main difference between the two systems is in the location of the recycle of methane and oxygen back to the reactor. The recoveries of key components and the composition of the product streams for process 1 and 2 are shown in table 4.6 and 4.7 respectively.

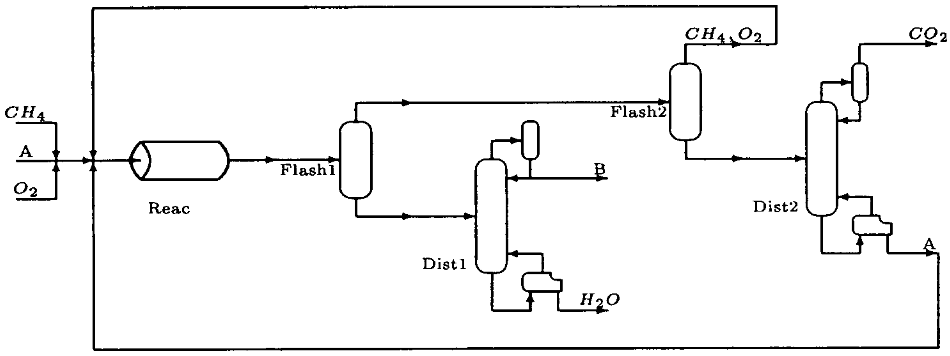


Figure 4.11: Environment Study, Process 1

Unit	LK	Recovery
Flash1	A	0.88
Dist1	B	0.99
Flash2	CH_4	0.80
Dist2	CO_2	0.96

	Flue	Product	Sewage
CO_2	34.4	0.0	0.0
O_2	0.0	0.0	0.0
CH_4	15.6	0.0	0.0
B	0.0	80.3	0.8
A	4.3	14.6	0.0
H_2O	0.0	0.7	68.2

Table 4.6: Process 1, Recoveries and Product Composition

The energy requirements of both systems are similar but the stream compositions leaving the system are different, therefore determination of the environmental impact

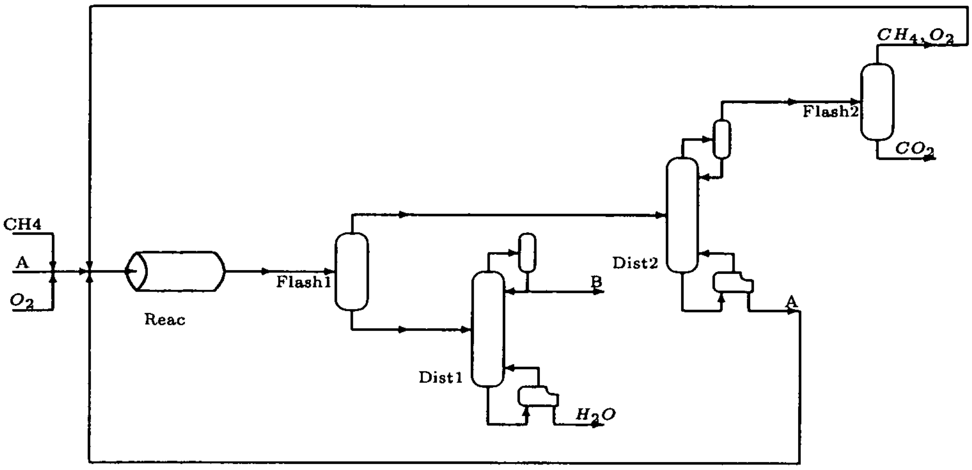


Figure 4.12: Environment Study, Process 2

Unit	LK	Recovery
Flash1	A	0.88
Dist1	B	0.99
Flash2	CO_2	0.90
Dist2	CH_4	0.85

	Flue	Product	Sewage
CO_2	36.9	0.0	0.0
O_2	3.9	0.0	0.0
CH_4	13.1	0.0	0.0
B	0.0	75.5	0.8
A	10.0	13.7	0.0
H_2O	7.4	0.7	73.0

Table 4.7: Process 2, Recoveries and Product Composition

of the streams leaving the process needs to be assessed. It has been decided that the primary concern for this process is the global warming potential. The values of the global warming potential of each component are shown in table 4.8 and are stored in their respective component `component statistic` objects. The final destination of the stream determines which of the indices will be used.

	CO_2	CH_4	O_2	H_2O	A	B
Green House	1	11	0	0	800	1600
Flue Green House	1	1	0	0	200	200

Table 4.8: Global Warming Potential of Components

The environmental study can then be applied which gives the results shown in table 4.9 for the contribution to greenhouse warming potential.

	Process 1	Process 2
Feed	268.5	268.5
Product	1466.3	1464.8
Flue	16.7	16.5
Sewage	18.8	34.3
LCA	1233.3	1247.1
Substitution/Elimination	1.024	1.035

Table 4.9: Environmental Index Results

The life cycle assessment reflects the most accurate assessment of environmental impact and from this analysis it can be seen that process 1 is slightly more favourable to process 2. The results show that the small difference between the two processes is due to the sewage stream. The environmental impact of process 2 could be improved by attempting to reduce the impact of this stream or adding on further treatment processes. However, a low substitution/elimination index for both processes shows that potential improvements to the process are unlikely and any remedial action is likely to involve end of pipe treatment.

4.4 Pipe Size

Pipe sizing while not a process ranking index in itself, is used by many of the other indexing procedures and demonstrates the need for the package to have the ability to interface to other packages. The chemical exposure index requires knowledge of the size of pipe work attached to each process unit, and the layout program requires information about the costing of the pipe work, which is related to pressure and diameter of a pipe. The pipe size package is an evaluation tool which helps the designer identify areas of interest where extra design considerations are likely to be required. The system has to have the ability to perform physical property calculations to evaluate the volume of flow of a stream and report back the calculated area and diameter.

4.4.1 Assessment Method

The pipe size evaluation is performed over the entire topology on a stream basis. From each `stream` object the temperature, pressure, phase, and component flows are extracted. If the `stream` has a `statistic` object associated with it then it is examined to see if it contains a 'volumetric flow' and a 'speed of flow' slot. If these values are known then the calculation of pipe diameter is a simple procedure, otherwise the physical property of the stream needs to be examined.

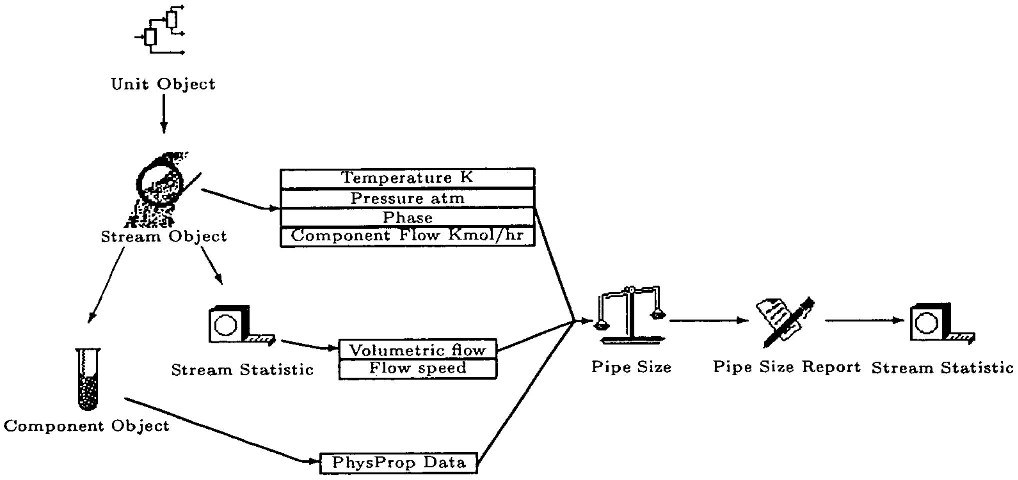


Figure 4.13: Formation of the Pipe Size Assessment

Figure 4.13 shows how all of this information comes together to formulate the pipe size. If the stream statistic does not contain speed of flow information, then for a liquid it is assumed to be 5 m/s and a gas 20 m/s. If the volume of flow is unknown then the system needs to extract the physical property data from each component and evaluate the molar liquid or molar gas volume. The post synthesis package has access to the same physical property package as that available during synthesis. So if the standard volumes of a mixture have not been calculated at the synthesis stage then they can be calculated and returned to the stream statistic for use at a later date.

Once the molar volumetric flow is known along with speed of flow, the system can calculate the diameter of the pipe work. The values of diameter and area can then be returned back to the `stream statistic` to allow for further post synthesis methods to be carried out.

4.5 Steady State Control Analysis

Integrating control concerns is one of the most difficult aspects of design. Identifying designs that are difficult to control and measuring this extent can prove problematic especially with the absence of a control structure. Designing a process which lends itself as being easy to control can improve the profitability of a process and increase system safety. Steady state analysis provides the simplest form of analysis and aims to establish if a process is possible at varying operating conditions. The extent of which is measured by a flexibility index, where perturbations are made to the system, until the system becomes unfeasible.

It is useful to make to make the distinction between the three operability measures flexibility, controllability and reliability of a process. Flexibility is the ability of a process to reject a disturbance and ensure feasible regions of operation (Grossmann et al. [50]). Controllability is a measure of how difficult a process can be to control and is a measure of the quality and stability of the dynamic response of the process (Lennhoff and Morari [51]). Reliability is concerned with the probability of normal operating given that mechanical and electrical failures can occur. Reliability tends not to be dependent upon the inherent characteristics of a process and a final design can usually be tuned to achieve a specified reliability by incorporating redundancy into the design.

4.5.1 Flexibility Index

Flexibility is a major concern in the design of a chemical plant. Synthesis is usually set to find the most optimal design for one operating condition. It is highly unlikely that a process will operate at one throughput and it is essential to find out how much disturbance a process can tolerate. This is especially important with design that has to handle multiple feed stocks. Disturbances can take a variety of different forms including changes in ambient conditions, feed stock changes, fouling of heat exchangers etc.

Controllability and flexibility measures tend to be linked so that if a process is highly flexible then it tends to be easier to control. However, the converse is not necessarily true as an easily controlled process is not an indication of a flexible process. An example of this would be with a shell and tube heat exchanger where one or two parallel heat exchangers can be used. The parallel case would be unable to reject disturbances as well as the single larger exchanger, but a smaller lag time in the parallel case will result in a process which is easier to control.

4.5.2 Control Flexibility

Grossmann [50] defined flexibility as 'The problem of ensuring the existence of feasible regions of operation for a variety of different conditions'. He has proposed optimisation strategies for chemical processes and these have been developed by Padley [17] incorporating them into process synthesis. Grossman has described two objectives which can be applied when designing a chemical plant. They either design for a fixed degree of flexibility at minimum cost or obtain an optimal degree of flexibility that is actually required by the process. Satisfying the second objective requires a multi-objective analysis to be performed to establish the trade off between flexibility and cost, and hence requires an index of flexibility.

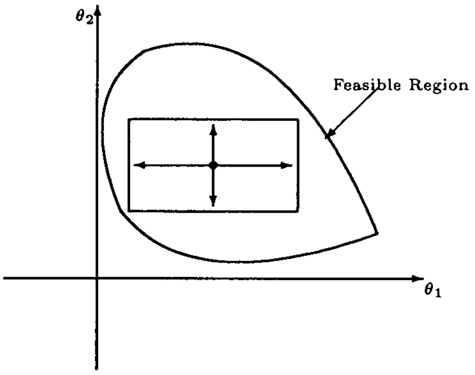


Figure 4.14: Feasible Region and Inscribed Hyperrectangle

A strategy for flexible process design has been proposed by Grossmann et al. [50] and developed into an index for operational flexibility [52] and respective computational algorithms [53]. The index analyses a set (p) of uncertain parameters θ_i i=1,..p. Figure 4.14 shows the feasible region of a process for 2 parameters.

In order to find the flexibility of a process it would be useful to find the boundaries of feasibility. However, it is difficult to find these boundaries, visualise them in more than two dimensions and return a single meaningful result. Therefore the approach of inscribed hyperrectangles is used.

It makes sense to analyse around the normal parameters which must lie within the feasible region then perturbations can be made to the system until it becomes infeasible. The system can be examined at the extremities of each combination of disturbance. Geometrically this corresponds to inscribing the feasible region with a hyperrectangle with a centre at the normal operating point.

The user has to decide how to expand the rectangle and this is dependent upon the degree of variance expected. The search can then proceed until an apex is found which violates the feasible operation. Grossman [52] proposes scaling according to expected deviations therefore reducing the hyperrectangle to a hypercube. With the flexibility being half the length of one of the sides of the cube.

While this is useful for visualisation purposes a search can be carried out by gradually expanding the hyperrectangle in proportion to the expected deviations. A coarse search is carried out until two points either side of the feasible region are found then a bisection search is carried out to find the exact bounding position. A flexibility index can therefore be returned depending upon the amount of expansion required from the expected deviations. A flexibility index greater than 1 indicates that the system can handle deviations greater than expected.

It is possible to have a system which has more than one critical point. The system shown in figure 4.14 is convex and the solution must lie at one the vertices of the hyperrectangle. Grossman [52] has also shown conditions required for a vertex solution in a non-convex solution space. The non-convex space and maximum hyperrectangle is shown in figure 4.15. The method of analysis to find if the space is non-convex is done

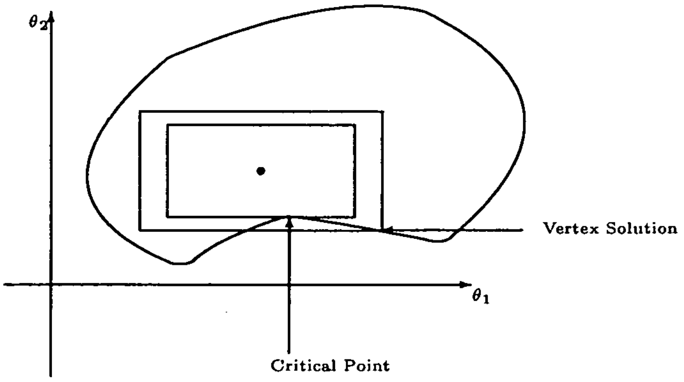


Figure 4.15: Non-convex Feasible Region and Inscribed Hyperrectangle

by searching for parallel lines to to the apex solution and examine if they cross feasible space. For practicable purposes the method of analyses is to search along the edges of the hypercube to find points of infeasibility, if this occurs then the hyperrectangle can then be scaled to fit. However, for the purpose of conceptual design we will be working with linearised models and the solution space will never be non-convex.

A steady state linear model of a process can be generated and the system modelled in Matlab [54]. Possible disturbances to the system are identified and the user can select which disturbances they wish to examine and the magnitude of the expected disturbance. Modelling with a linearised system enables quick calculations to be carried out and can be easily determined from the topology of the system. Linearised models tend only be valid for small disturbances around the normal operating parameters. They cannot cope with pinch constraints caused by heat integration and if pushed too far may create negative component flows. If a constraint is close to the normal operating parameter it can be a cause for further analysis to be carried out upon the system around that point.

Using Matlab enables an output file to be generated by the system which is self contained including the input data and the method of analysis. The user can easily edit this file as the design progresses and if the Web browser is set up correctly can call Matlab directly. Matlab allocates variables, performs error exception and has a number of useful mathematical tools such as sparse matrix handling available. The compromise is a small loss of speed that would be expected compared to the development of a dedicated analysis tool.

4.5.3 Flexibility Development Study

The flexibility index can be demonstrated with the following development study. Two processes are available depending upon the type of catalyst used. Catalyst 1 takes components A and B has an 80 % conversion and produces product P. Catalyst 2 has a higher conversion of 92 % but also has a secondary reaction which decomposes the product to produce a waste product W shown in equation 4.27. A product purity greater than 98 % of B is required and therefore the two systems have a sharp separation system with a recovery of 96 % and 90 % respectively.

$$\begin{array}{c} A + B \rightarrow P \\ P + B \rightarrow 2W \end{array} \tag{4.27}$$

The topology of both systems is shown in figure 4.16 along with the component molar flow rates. Both systems produce the same product stream.

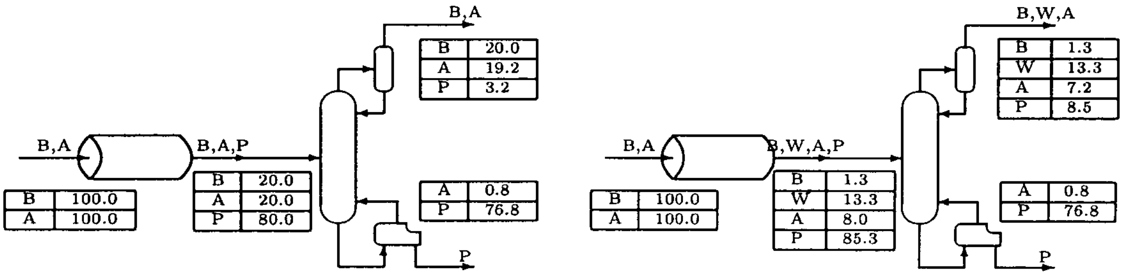


Figure 4.16: Flexibility Development Case Study Topology

Potential disturbances to the system are the feed flow rate of each component, the conversion of each component and the recovery in the separation section. The model

	Process 1		Process 2	
	Original Value	Displaced Value	Original Value	Displaced Value
Light Key Recovery	0.960	0.927	0.900	0.841
Heavy Key Recovery	0.960	0.927	0.900	0.851
Feed A kmol/hr	100.0	100.7	100.0	101.2
Feed B kmol/hr	100.0	99.3	100.0	98.8
Flexibility	0.66		1.19	

Table 4.10: Flexibility Development Study Results

of the process is a linear system and disturbances have to be kept small to ensure that the model remains feasible. In this situation we can expect a 1 kmol/hr disturbance in the feed flow of each component and a recovery variation of 5 % . The only constraint placed upon the system is to maintain the product purity P.

The results of the flexibility study are shown in table 4.10. With the expected deviations process 2 has a better flexibility than process 1. For both processes the limiting factor is the quantity of A present in the system. An increased amount of A and a lower recovery result in a system result in failure to make a specification product. To ensure that the analysis is correct a complete model of the reactor needs to be formulated[4] about the point of infeasibility.

The flexibility index is dependant upon the expected deviations from the normal operating parameters. If the deviation in flow is expected to double to 2 kmol/hr and the expected deviation in recovery to half to 2.5 % then the flexibility for process 1 is 1.13 and bounded by the process constraint and 0.65 for process 2. However, the flexibility of process 2 is bounded by negative flows caused by excessive reactor conversion. This is an indication that the linearised model has been pushed too far and is therfore not valid for this analysis. Analysis of the true conversion from the reactor at the corners of the hyperrectangle can be carried out and the flexibility analysis can then be repeated if these points are feasible.

---

[4] Increasing the complexity of the reactor model can change the search space from convex to non-convex.

4.6 Dynamic Control Analysis

Dynamic analysis is the most complicated control analysis to perform as it allows for the interaction between units over time to be examined. There are two methods of analysing the dynamic response of the system. The first works around a linearised approximation of the system using the steady state gains of the system and its time response. The second method uses a full dynamic model of the system, and the response of the system is evaluated at a discrete number of time steps. Linearised approximation to the system has the advantage that the response can be quickly evaluated, but only small perturbations can be made to the system and small compounding interactions may be neglected. A full dynamic simulation allows for a greater range of conditions to be examined including startup and shutdown, but the complexity of the system can result in an analysis that is computationally expensive. Dynamic simulation also requires a comprehensive knowledge of the system to be modelled including the correct selection of physical property data and operating conditions. At the conceptual stage of design much of this information is unknown and to perform a successful simulation extensive user input has to be used. Linearised approximations can reduce this level of input by the user, and has the most potential for quickly assessing conceptual design. However, the linearised model should be consistent with the dynamic simulation, and we intend to compare the two methods through a development study.

The strengths and applicability of the two methods to conceptual design will be examined.

- The resilience of a linearised approximation of the system based around the steady state gains of units and the units time response.
- The resilience of a dynamic simulation involving the units control structure and the response of each unit.

4.6.1 Process Resilience

During process design decisions about the process structure can affect the operating characteristics. For example the sequencing and number of distillation columns, reactors etc. along with their heat integration can produce operating conditions that are undesirable. When process materials and utility costs were cheap a disjointed process structure would be common and individual process units could be assessed. With process integration now more common in process design a quantitative measure of the resilience of the plant is required early on in the system of design. Heuristics have been proposed to deal with this problem, but these have proven to fail to produce resilient processes in certain situations, or they conflict with techniques for heat integration and process layout. Resilience is defined as to how quickly and smoothly the system will move from one operating condition to another and deal with disturbances.

For the purpose of this analysis we will assume that,

- Certain measures are to be kept at a desired level or they should follow a time varying reference.
- Not all of the disturbances on the plant can be measured, therefore the use of feedback control is necessary.
- All of the beneficial feed-forward loops have been implemented.

Resilience assessment will show the quality of control that can be obtained. Resilience assessment can assess either individual process units but more importantly their interactions between each other.

4.6.2 System Definition

A controllability assessment should be able to assess which of the process structures are to be carried forward for further analysis. The analysis is not aimed at providing a formal control structure to the system, but rather to analyse the process structure and highlight where difficulties in control may exist, so that beneficial process systems can be developed further.

Control measures typically depend upon the plant design, the type of controllers, the operating conditions and the type of controllers employed. A typical method to assess the controllability of a system is to select a control structure to apply to the system, and then tune the controller to optimal. This gives an assessment as to the system under closed loop control. But it is desirable to have a method that can be performed in reasonable time, and does not rely upon the existence of a control structure. The method formulated for resistance analysis by Morari [55] can be used where the problem is approached with the insight that the ultimate closed loop behaviour is determined by constraints in the system. Some of the constraints are obvious such as reactor size which restricts the amount of conversion possible or valve size which constrains the total flow possible. This allows the assessment of the system independent of the controller type. Assessment of the plant can be made with respect to perfect control using the following indexing methods.

- The minimum squared error between the set-point and the output.
- The minimum time for the closed loop system to reach steady state.

In order to understand the inherent characteristics which limit controllability it is important to understand the nature of feedback control. To do this it is assumed that the system can be represented by the transfer matrix $G(s)$, i.e.

$$y(s) = G(s)u(s)$$

If we employ the feedback structure as shown in figure 4.17, we can split the plant into its inputs and outputs. Inputs to the system can be broken down into outside inputs (a) and controlled inputs (b). Outputs from the system are regulated outputs (c) and sensor outputs (d) such that.

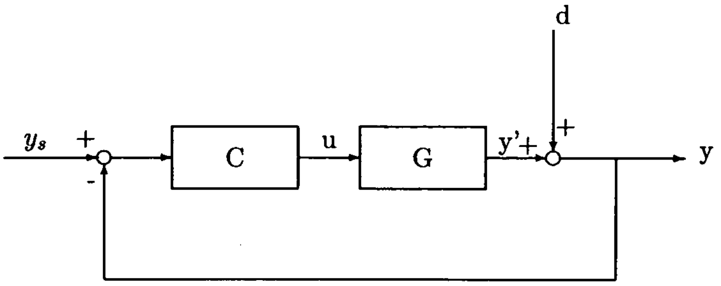


Figure 4.17: A typical feedback control structure

$$\begin{bmatrix} c \\ d \end{bmatrix} = G \begin{bmatrix} a \\ b \end{bmatrix}$$

Outside inputs to the system would be inputs that can either not be measured or are unknown disturbances. In the case of a distillation column this could be feed composition. For the controlled inputs the system could have control over the feed flows into the system. Regulated outputs are outputs that the system creates, these in turn may affect further process units. Sensor outputs are the objective control outputs such as the product composition. The main advantage of this system is that feedback control is taken regardless of the source of the disturbance.

The feedback control structure shown in figure 4.17 is for a single input single output system (SISO). Morari [55] has shown that perfect control is only possible if $G(s)$ has a right inverse which is shown to be true in appendix C. The same analysis can also be applied to a mixed input mixed output system. For any system the following observations can be made.

- A feedback controller provides an approximate inverse of the plant transfer matrix, from sensor outputs to controlled inputs.
- Closed loop control quality is limited by the system invert-ability.

In the early stages of design examining the transfer matrix will point the designer to suitable manipulated variables. It is desirable to perform resilience analysis in the

Laplace domain with $n * n$ matrix for $G(s)$. It is therefore possible to gain a general understanding as to the control behaviour of the system.

Once the transfer function of a system is known then analysis tools can be applied which can analyse the response of the system. In particular Matlab [56] has a control package available which enables transfer functions to be attached together, their response examined and for control systems to be developed.

The first question that needs to be examined is can a perfect controller be implemented. The ability to implement a perfect controller is dependent upon the relationship of poles and zeros in the transfer function. Poles occur where values of the transform variable s occur that cause the transfer function to become infinite and at points where roots of the denominator of the transfer function are common to roots of the numerator.

Zeros occur where values of the Laplace transform variable s occur that cause the transfer function to become zero, and at points where the roots of the numerator of the transfer function are common to roots of the denominator.

For example $\frac{s+2}{s(s+5)}$ has a pole at 0 and -5 and a zero at -2.

If we assume that we want to install perfect control then a measure as to how far away from this is possible would give an indication to the controllability of the system. Morari has shown that the three conditions that make perfect control impossible are:

- The number of zeros exceeds the number of poles in G^{-1}, resulting in infinite controller power for implementation.
- If G contains time delays, then predictive elements would have to be present in G^{-1}.
- If G contains right hand plane zeros which then become unstable in G^{-1}.

Examination of the transfer function will give an indication as to which of these conditions apply. If the system invert-ability is limited by the position or location of a zero then we could expect the system to be unstable resulting in a difficult control problem. If perfect control is limited by time delays then an imperfect controller can be created. The limitations upon the controller are governed by the magnitude of the time delay and the system response.

For the purpose of generality we are going to look at both SISO and MIMO systems.

4.6.3 Control Analysis Method

An extension to the management system has been developed to record the control structure used. A `control` object has been developed which is similar to a `topology` object with slots for transfer function inputs, outputs and intermediate functions. The overall structure is held together with a control structure topology, therefore allowing complicated systems to be developed. The structure can also be linked across units and is not dependent upon the process topology. Information about the transfer functions are kept in `transfer function` objects and contain slots for numerator and denominator values of the transfer function.

The analysis package collects all of this information and formulates a Matlab input file where the response of the system can be analysed.

4.6.4 Control Examples

To demonstrate the use of control structures two development case studies are shown. The first shows a surge tank and the development of the transfer functions. Then linking these tanks in series or parallel to determine which provides the most resilient design. A distillation column is then studied and the resilience of the sequencing of two columns is examined.

4.6.5 Surge Tank

For a surge tank system, we may want to examine how the outflow from one tank relates to changes in the input $Q_i'(s)$. The outflow from the tank is linearly related to the height of the liquid.

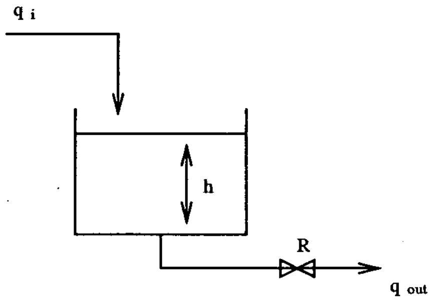


Figure 4.18: Single surge tank system

Assuming that the outflow valve resistance R is fixed, we can write the following equations for the system.

$$A\frac{dh}{dt} = q_i - q_{out} \tag{4.28}$$

$$q_{out} = \frac{1}{R}h \tag{4.29}$$

A transfer function relating $H'(s)$ to Q'_{out} by substituting, transforming and rearranging equations 4.28 and 4.29 to give.

$$\frac{H'(s)}{Q'_{out}(s)} = \frac{R}{ARs+1} = \frac{K}{\tau s+1} \tag{4.30}$$

Equation 4.29 can be transformed to give.

$$\frac{Q_{out}(s)}{H'(s)} = \frac{1}{R} = \frac{1}{K} \tag{4.31}$$

This then gives the block diagram transfer function model.

To examine the effect of adding systems together, either in parallel or series, a transfer function of unity will have to be introduced. For example surge tanks in parallel can be represented by by the combination of transfer functions shown in figure 4.20.

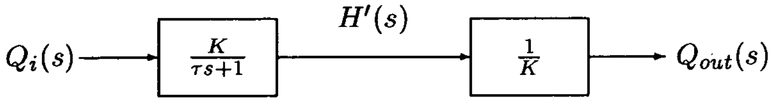


Figure 4.19: Surge Tank Transfer Function

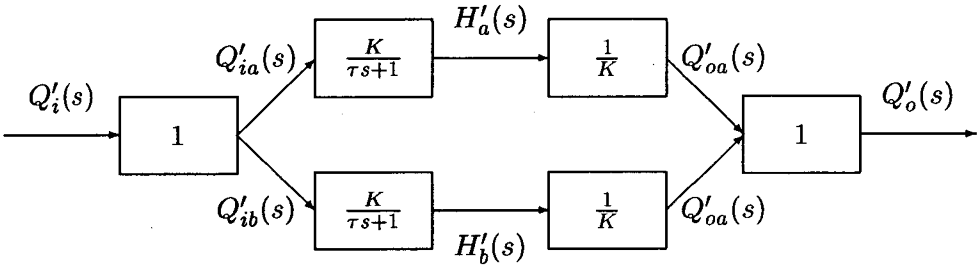


Figure 4.20: Transfer Function For Parallel Surge Tank

The multiplicative property of transfer functions allow us to build complicated systems of process units and instrument systems to be built. The overall system complies with the three rules for a perfect controller to be implemented and the system is limited by system constraints.

Tank Sequencing

The surge tank system can be used to examine the effect of coupling systems. Suppose there are 2 tanks as shown in figure 4.18 which are linked in series or a set of tanks with half the area linked in series. We would like to examine how many smaller tanks are required to produce a system that is more resilient than the 2 tank system.

For this purpose we will have to examine the effect of a step and an impulse on the system. For the system to be more resilient it must settle down in less time than the 2 tank system, and it must produce less of an error between the set point and the output for the system.

Results from the system can be obtained by linking together a number of tanks together

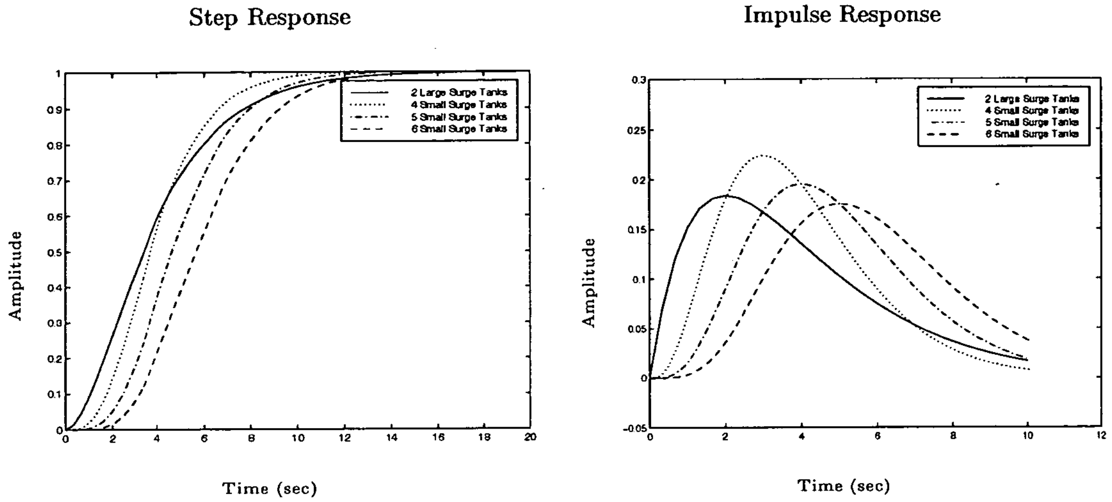


Figure 4.21: Surge Tank Response

and examining their response. We can examine the response of the system with respect to a step and an impulse on the feed flow. The results are shown in figure 4.21 for 2 large tanks along with 4,5 and 6 smaller tanks in series.

The resilience of the system can be examined by calculating the time taken for the system to move from one state to another and its ability to reject disturbances upon it. With the surge tank system the fewer the number of smaller tanks the quicker the response to a change in the system, with 5 smaller tanks approaching the resilience of the 2 large tank system. However looking at the impulse to the system we can see that more smaller tanks are required in order to reject disturbances placed upon the system. In this situation 6 tanks would be required to reduce the amplitude to a level below that of the large tank system.

We can see from this analysis that we cannot make a decision as to which set of systems is more resilient to changes in the feed flow. In order to identify which system is more resilient it is necessary to specify the objectives on the system. If in the case of surge tanks the objective is to remove disturbances on the system then the value of the minimum squared error between set-point and the output can be examined. Therefore looking at the impulse response 6 small surge tanks would be required for a more resilient system.

Distillation Sequencing

A distillation column can be modelled with a simplified linearised model. Most distillation systems contain time delays, and can take considerable time to achieve steady state. Distillation columns also have a number of points where disturbances can enter the system. They can be physically constrained in their operating parameters and a disturbance can have unexpected side effects.

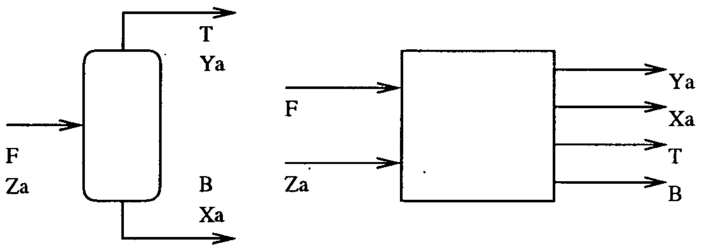


Figure 4.22: MIMO for distillation column

Considering one distillation column as shown in figure 4.22 with 2 disturbances on the feed flow and the feed composition we produce variations in 4 outputs. The transfer function employed for this system ignoring time delays is.

$$\begin{bmatrix} Xa \\ Ya \\ T \\ B \end{bmatrix} = \begin{bmatrix} \frac{0.07s}{s^2+0.2s+1.01} & \frac{1}{5s+1} \\ \frac{-s}{s^2+s+4.25} & \frac{3}{5s+1} \\ \frac{1}{2s+1} & \frac{1}{3s+1} \\ \frac{1}{0.5s} & \frac{1}{s+1} \end{bmatrix} \begin{bmatrix} F \\ Za \end{bmatrix}$$

Design restrictions in the output concentrations from one of the distillation column streams, where the feed composition to the system can be controlled will result in the system shown in figure 4.23. This will then produce the system,

$$Xa = \frac{0.07s}{s^2+0.2s+1.01}F + \frac{1}{5s+1}Za$$

The analysis of one distillation column will give only the basic input-output information. However, the system does allow linkages to be made across units such that the top or bottom products from 1 distillation column can be fed into another column and the

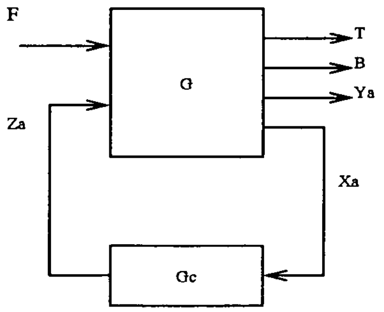


Figure 4.23: Single Column Distillation System

system analysed. If it is desirable to maintain the composition of 1 product stream this would then give 1 sensor output, 5 regulated outputs, 1 outside input and 1 controlled input.

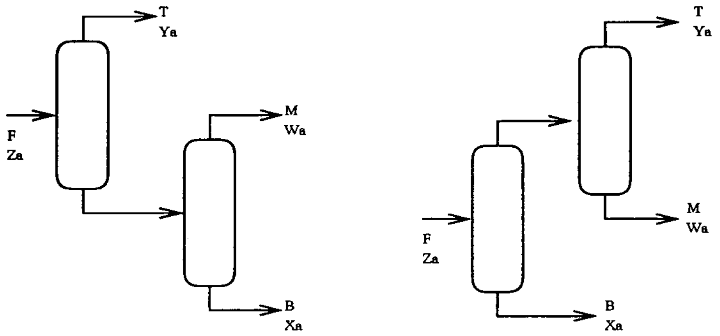
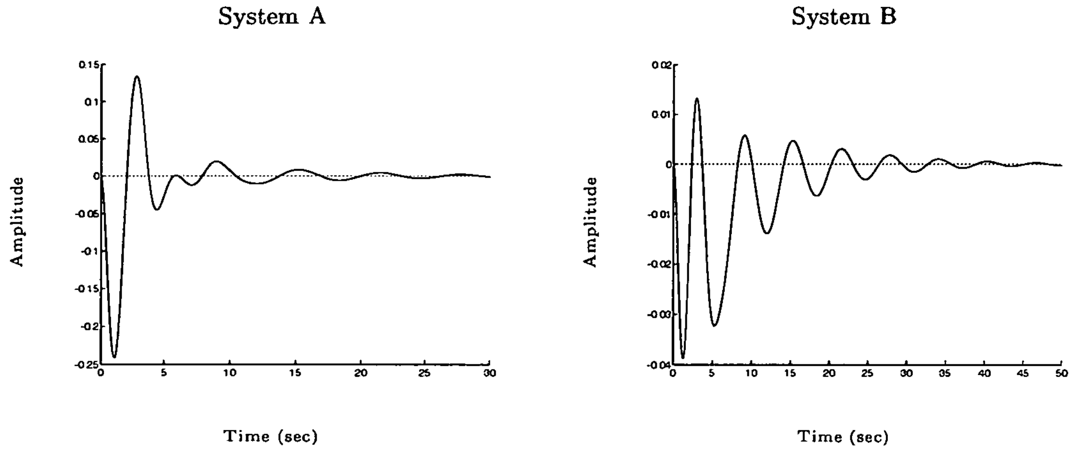


Figure 4.24: Distillation Column Sequencing

Distillation Sequencing

From the sequence of columns shown in figure 4.24 we have 3 compositions that we may wish to control. Supposing the principle concern is to control the middle composition Wa, we will want to examine the responses of Wa with respect to variations in F and Za.

The system is set up to return a graphical response of the system to a step response in the inputs to the system. Numerical information is also returned about the final value achieved, the percentage over the final value that the system will achieve, the time to reach 90% of the final value and the time for the system to settle to ±2% of its final value.



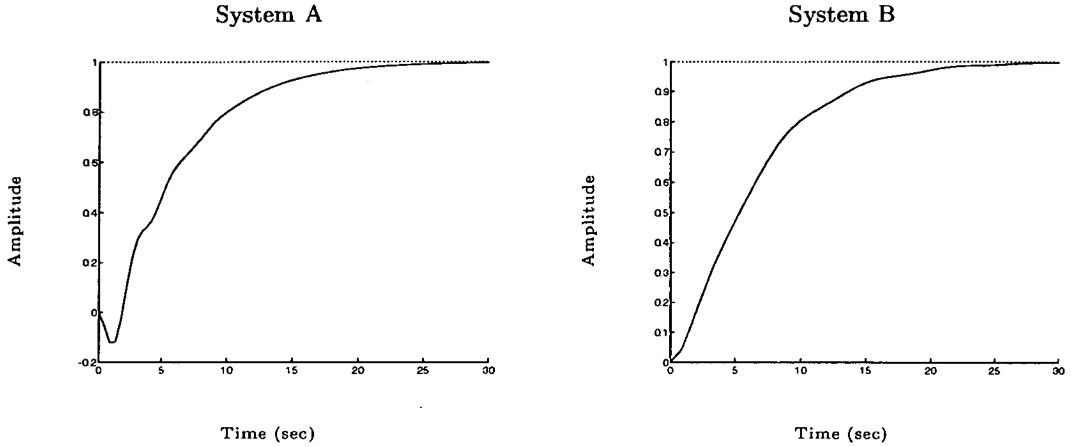
Final Value = 0
Percentage Over = Inf
Rise Time = 3.21
Settling Time = 23.72

Final Value = 0
Percentage Over = Inf
Rise Time = 3.75
Settling Time = 41.89

Figure 4.25: Wa response to a step in F

We can see that the output concentration Wa of both systems behave differently with respect to a step in the feed into the columns. Both systems exhibit an inverse response to the step change. System A settles down about 24 seconds after the change is made, whereas system B takes 42 seconds. This is partly due to the hold up in the reboiler of the first column, stabilising the effect of the change on the second column. The other criteria we have to assess resilience is the minimum squared error between the set-point and the output. In this case both of the systems return to their original value and therefore the minimum squared error is zero. We can also see that trying to control the output concentration Wa with the feed flow would be impossible. Comparing both systems we can see that system A is the more resilient process to changes in the feed flow.

Applying a step increase to the feed Za there is little difference between the outputs of the two systems, with both systems settling down to the same final value of 1. The settling time for both systems is similar. By plotting the response of the system we are also able to see any unusual behaviour. In this case system A has an initial inverse response to the change in Za. This is because an increase in Za leads to an increase in the bottom flow rate, which initially reduces the output concentration Wa from the



Final Value = 1
Percentage Over = NaN
Rise Time = 14.87
Settling Time = 24.21

Final Value = 1
Percentage Over = NaN
Rise Time = 13.84
Settling Time = 24.23

Figure 4.26: Wa response to a step in Za

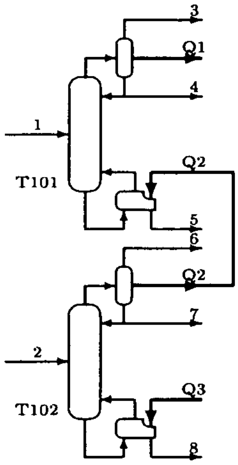
second column. There is little difference between the resilience of each system with respect to changes in the feed concentration.

4.6.6 Control of Integrated Process

Identifying differences in processes which contain recycles and heat integration is one of the main interests of post synthesis analysis. Synthesis can produce processes that differ only in the manner that they are heat integrated. Different heat integration can produce difficulties in the control and operation of each process. It would therefore be useful to have a method of assessing the controllability of a system.

4.6.7 Integrated Control Development Study

In order to demonstrate the controllability issues a development study has been chosen using two binary distillation columns to separate two feeds of propane and butane. Some controllers to maintain system pressure and liquid levels are assumed to be present. The feed compositions of the two columns and the operating pressures have been chosen so that a viable heat integration between the reboiler and the condenser can be made. Figure 4.27 shows the 2 columns with heat integration including the operating parameters. The re-boiler duty of T101 is supplied exclusively by the condenser of T102, therefore removing 1 degree of freedom in the control of both columns.



Feed	1
i-Butane	0.7 mole frac
i-Pentane	0.3 mole frac
Pressure	71 kPa
Temperature	-9 C
Flow	45 kgmole/hr

Feed	2
i-Butane	0.8 mole frac
i-Pentane	0.2 mole frac
Pressure	455 kPa
Temperature	42 C
Flow	56.5 kgmole/hr

Column	T101
Number of Stages	5
Feed Stage	3
Operating Pressure	490 kPa
Overhead Vapour Rate	0 kgmole/hr
Distillate Rate	32 kgmole/hr
Reflux Rate	193 kgmole/hr
Bottoms Production Rate	14 kgmole/hr
Boil Up Ratio	14

Column	T102
Number of Stages	16
Feed Stage	8
Operating Pressure	788 kPa
Overhead Vapour Rate	0 kgmole/hr
Distillate Rate	46 kgmole/hr
Reflux Rate	193 kgmole/hr
Bottoms Production Rate	10.5 kgmole/hr
Boil Up Ratio	20

Figure 4.27: Development study with 2 heat integrated columns

Steady State Model

All dynamic analysis is based on knowledge of the steady state system. The system can be modelled using a set of linear equations or through the use of a modelling package. The system shown in figure 4.27 is modelled in Hysys and the results shown in table 4.11.

Stream	4	5	7	8
Mole Frac (i-Butane)	0.985	$1.8 * 10^{-2}$	0.974	$7.9 * 10^{-5}$
Mole Flow	32	13	46	10
Temperature C	-20	16	33	77
Pressure kPa	69	69	422	422

Table 4.11: Steady State Results

Linearised Approximation

A model of the dynamic behaviour of a binary distillation column has been developed by Wahl [57] where approximate transfer functions describing the behaviour of the system are produced. The dynamic behaviour is characterised by parameters T_s and L_R obtained from knowledge of the steady state conditions.

T_s Time constant based upon the average concentration in the column. Which is dependent upon the number of plates, concentration and relative volatility of the components.

L_R Reduced circulation rate, and represents the extent of the column maintained at equilibrium.

This means that a system with a high circulation rate compared to the holdup of the column will maintain itself close to equilibrium and the output state of the column will be close to the input conditions.

In order to evaluate the time constant and the reduced circulation rate information about the column needs to be present. Including the number of plates, product composition, relative volatility, reflux ratio, plate holdup, reboiler holdup, condenser holdup, and the minimum reflux rate. Most of this information is held in the `unit` object or can be evaluated using the physical property package. `Stream` objects connecting to the `unit` can be used to identify the key components and hence their relative volatility.

Disturbances can enter each column through four possible load points: (1) the feed composition, (2) the feed rate, (3) the boil-up rate and (4) the reflux rate. The dynamic analysis is based around a stage wise model and therefore the temperature of the feed is not considered as it effects the reflux and boil-up of that stage and hence the overall reflux and boil-up of the condenser and reboiler.

Wahl [57] has described how a binary distillation column can be modelled using a number of parameters, and how to obtain each of these parameters. The method relies upon graphical interpretations of experimental results, however approximations can be made and the following process is used.

1. Evaluate $T_s = f(N, x_n, \alpha)$

   For a product composition mole fraction $0.9 > x_n > 0.99$

   and a relative volatility in the range $1.25 > \alpha > 2.5$

   Ts can be approximated by $T_s = \frac{N^{3.5}}{200+10N}$ $N = Number\ of\ plates$

2. Evaluate $L_R = T_s L / H_T$ where the total hold up $H_T = T_s * f$

   $f = feed\ flow$ and $L = Liquid\ Rate$

3. Evaluate T_1 using $\frac{T_1}{T_s} = 1 - \frac{1}{L_R^{0.75}}$

4. Evaluate T_2 using $\frac{T_s}{T_2} = 1.4(0.8 + L_R)$

5. Evaluate T_3 using $\frac{T_3 * V}{H_p} = \frac{N^{1.3}}{3}$ where the plate hold up $H_p = \frac{H_T}{N+3}$

6. Evaluate T_4 using $\frac{T_4 * V}{H_p} = \frac{N^{1.1}}{3}$

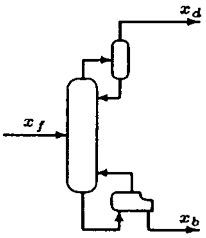
7. Evaluate T_z using $\frac{T_z - T_2}{T_2 + T_4} = 1.5 * Hf^3 - 1$ with fractional hold up $H_f = \frac{N}{N+3}$

Using this approximation the time response of the two columns T101 and T102 can be obtained and the results are shown in table 4.12.

A transfer matrix such as shown in equation 4.32 is obtained, with the recommended transfer functions shown.

	Column T101	Column T102
T_s	1.11 minutes	45.5 minutes
L_R	8.44	3.40
T_1	0.89 minutes	27.3 minutes
T_2	0.080 minutes	7.73 minutes
T_3	0.045 minutes	0.43 minutes
T_4	0.032 minutes	0.25 minutes
T_z	0.008 minutes	6.90 minutes

Table 4.12: Time Responses



$$\begin{bmatrix} x_d \\ x_b \end{bmatrix} = \begin{bmatrix} G_{11} & G_{12} & G_{13} & G_{14} \\ G_{21} & G_{22} & G_{23} & G_{24} \end{bmatrix} \begin{bmatrix} x_f \\ f \\ RefluxRate \\ BoilUp \end{bmatrix} \tag{4.32}$$

$$G_{11} = \frac{G_{xd}(T_z s+1)}{(T_1 s+1)(T_3 s+1)} \quad G_{12} = \frac{G_{fd}(T_z s+1)}{(T_1 s+1)(T_2 s+1)} \quad G_{13} = \frac{G_{Rd}}{T_1 s+1} \quad G_{14} = \frac{G_{Bd}}{T_1 s+1}$$
$$G_{21} = \frac{G_{xb}(T_z s+1)}{(T_1 s+1)(T_3 s+1)} \quad G_{22} = \frac{G_{fb}}{T_1 s+1} \quad G_{23} = \frac{G_{Rb}}{T_1 s+1} \quad G_{24} = \frac{G_{Bb}}{T_1 s+1}$$

The gain of the system is evaluated by using steady state calculations. These can either be evaluated using a linear model or using a modelling package such as Aspen or Hysys. $G_{xd}, G_{fd}, G_{Rd}, G_{Bd}$ represent gains in the distillate concentration with respect to changes in feed concentration, feed flow, reflux rate and boil up respectively. $G_{xb}, G_{fb}, G_{Rb}, G_{Bb}$ represent gains in the bottom concentration with respect to changes in feed concentration, feed flow, reflux rate and boil up respectively.

Time delays to the systems response can also be incorporated through the use of pade approximated transfer function. Time delays are dependent upon the size of the column and the output concentration and can be evaluated with the use of equation 4.33.

$$delay = \frac{3.T_s + 15}{5} \tag{4.33}$$

A linearised approximation can be made to the whole system, including the interactions between the bottom reboiler and the top condenser, which in this case are only weakly coupled. This results in a highly complicated system being generated, and therefore simplifications need to be made.

If it is assumed that a control structure will be applied to the column such that the reflux rate of the top column and the boilup rate of the bottom column is perfectly controlled so as to maintain the pressure of the system then transfer functions for these operations are not required. Also ignoring changes in the feed flow means that disturbances to the system can only enter through the input concentration to each column and into the other distillation column through the heat integrated reboiler-condenser. This results in only 4 transfer functions describing the behaviour of the system being required. Combining the heat integration of the system across the two columns the transfer function diagram shown in figure 4.28 is obtained.

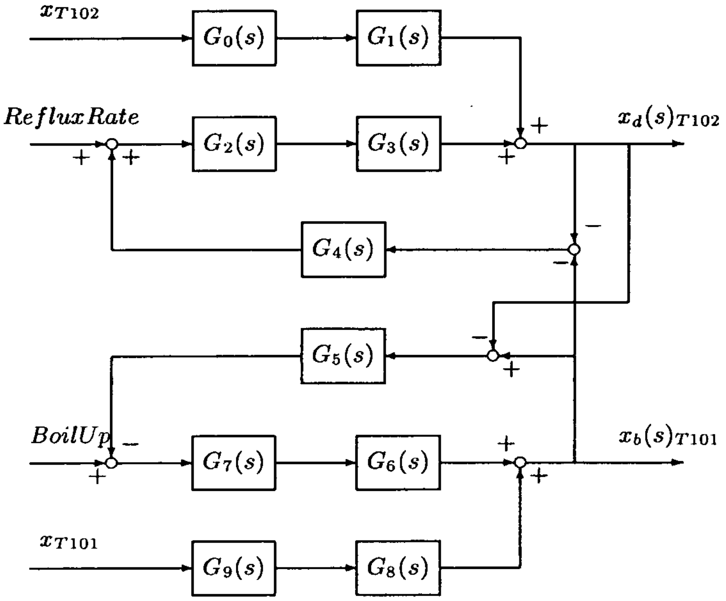


Figure 4.28: Transfer Function Diagram

x_{T102} = Feed concentration into bottom column T102.
x_{T101} = Feed concentration into top column T101.
Reflux Rate = Reflux Rate of bottom column T102.
Boilup = Boilup of top column T101.
$x_d(s)_{T102}$ = Distillate Product Concentration of T102
$x_b(s)_{T101}$ = Bottom Product Concentration of T101

$$\begin{array}{cc}
G_0(s) = \frac{-2s^3+6s^2-7s+35}{2s^3+6s^2+7s+35} & G_1(s) = \frac{0.068}{68s+1} \\
G_2(s) = \frac{-2s^3+6s^2-7s+35}{2s^3+6s^2+7s+35} & G_3(s) = \frac{0.0011}{68s+1} \\
G_4(s) = 1 & G_5(s) = 1 \\
G_6(s) = \frac{0.021}{127s+1} & G_7(s) = \frac{-93s^3+37s^2-6s+0.4}{93s^3+37s^2+6s+0.4} \\
G_8(s) = \frac{0.0002}{127s+1} & G_9(s) = \frac{-93s^3+37s^2-6s+0.4}{93s^3+37s^2+6s+0.4}
\end{array}$$

This structure along with the gains and the time responses produces a linearised model of the two columns which can be imported into Matlab. Gains for each transfer function can be calculated from steady state models. The system can then be examined to the influence of a step and impulse disturbance in the feed to both columns and the results plotted.

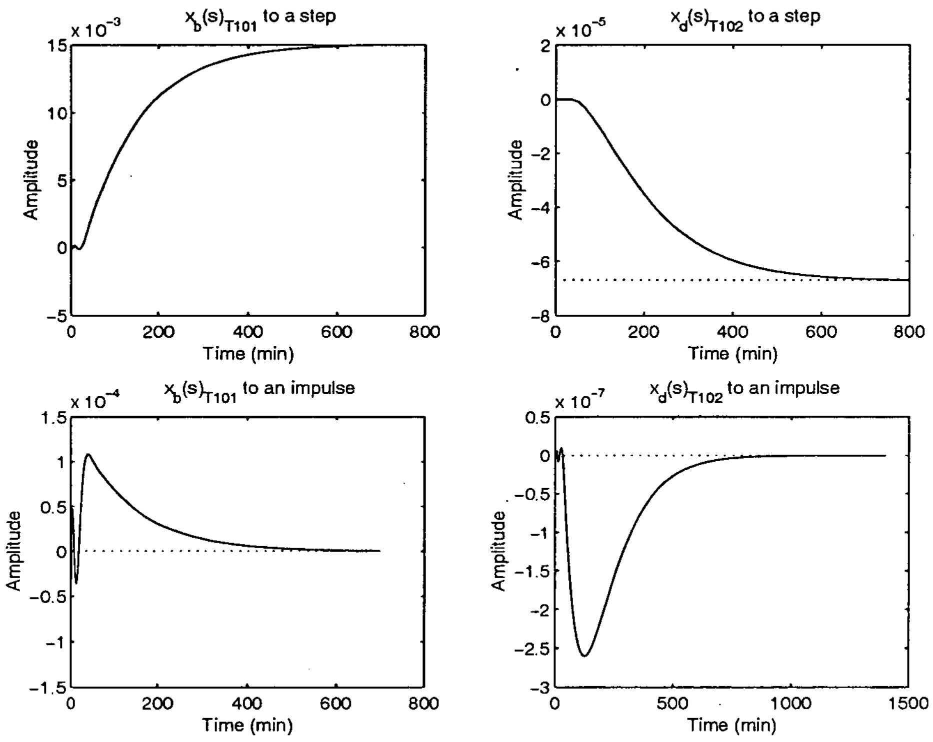


Figure 4.29: Disturbing the Feed of T101

Figure 4.29 and 4.30 shows the amplitude in the output concentration of i-Butane to a disturbance in stream 1 and 2 respectively. Where the disturbance on the input is a unity step and a unity impulse. Of particular interest is the effect that a change of concentration of the stream into a column has upon the output concentration of the other column and the graphs show the output streams of both columns from the heat exchanged re-boiler/condenser.

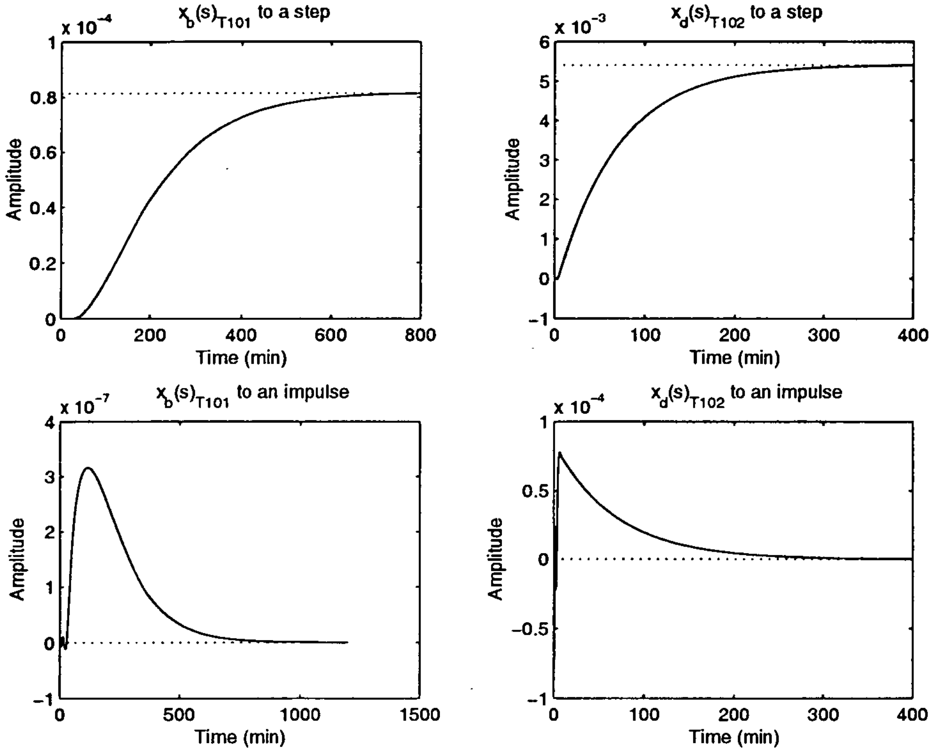


Figure 4.30: Disturbing the Feed of T102

As would be expected an increase in the feed concentration to T101 shown in figure 4.29 leads to an increase in the concentration leaving the bottom of the column. This analysis also shows that the time taken for the system to reach steady state being approximately 10 hours, which is an indication of a low circulation rate compared to the inventory held within the system. A small decrease in the output concentration from the distillate of T102 is also seen. The interaction between the columns can be explained by the fact that when the i-Butane concentration is increased in stream 1 the pressure in the column increases leading to a reduction in the condenser duty. This in turn leads to a reduction in the boil up in the column and also reduces the reflux rate of T102. Therefore a reduction in the output concentration from T102 is seen.

Figure 4.30 shows the effect of increasing concentration of i-Butane in stream 2. An increase in the feed concentration directly leads to an increase in the concentration of the distillate stream. Because the pressure of the column is maintained by reducing the reboiler duty which in turn reduces the reflux rate. The boil up in the top column

T101 is then reduced and an increase in the output concentration leaving the bottom flow is seen.

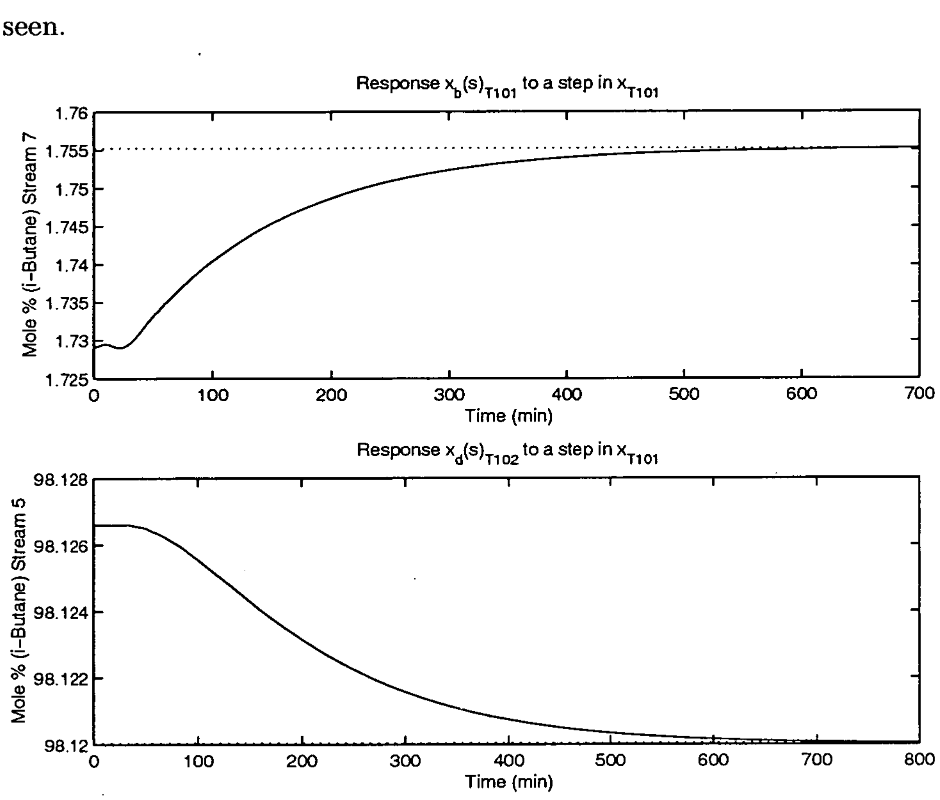
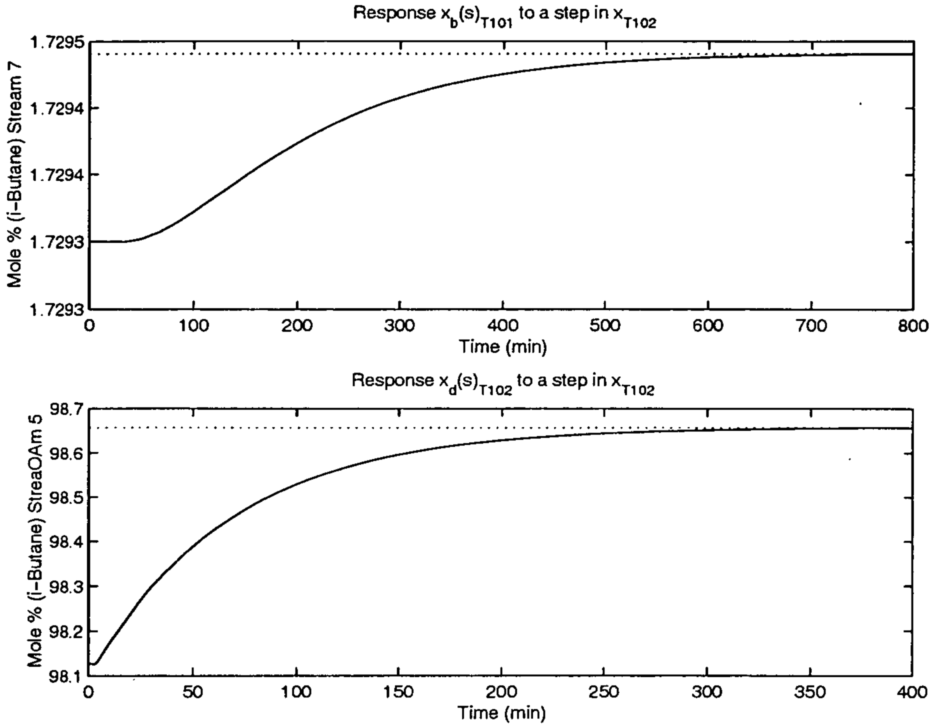


Figure 4.31: Composition Results to a Disturbance in Feed to T101

To be able to identify if this is cause for concern the actual concentration response needs to be examined. This can be done by examining the mole percentage of i-Butane from the bottom of T101 and distillate of T102 from a steady state model. The amplitude from the linearised model can be used along with expected input disturbances to give a prediction to the actual output concentration. Figure 4.31 shows the response of the system to a step increase in stream 1 of i-Butane concentration from 0.7 to 0.75. A similar analysis can also be carried out with a step increase in the concentration of i-Butane of stream 2 from 0.8 to 0.85 and the results shown in figure 4.32

From this analysis we can see that only small interactions occur between the reboiler and the condenser of the two columns. It could therefore be expected that a control system can be developed on an individual column basis with 1 degree of freedom removed.


Response $x_b(s)_{T101}$ to a step in x_{T102}

Response $x_d(s)_{T102}$ to a step in x_{T102}

Figure 4.32: Linearised Composition Results to a Disturbance in Feed to T102

This analysis only examines the interactions between units and does not examine the physical parameters of the units involved. For example, the analysis assumes that the top tray of a distillation column can tolerate small increases in the reflux rate without flooding occurring. In order to find out if this is a problem steady state resilience analysis needs to be carried out on the completed distillation design.

Creating a combined linearised model is a difficult task especially when trying to visualise the effect of each disturbance. The main advantage of this method is the short evaluation time required to evaluate the response of the system. In order to evaluate how accurate a linearised model is comparisons to a dynamic model have to be made.

Dynamic Simulation

Full dynamic simulation can be a very complicated modelling problem, with heat integration constraints and the interaction of different units having to be evaluated at each time interval. A comprehensive understanding of the system is essential before dynamic modelling can begin. Parameters such as vessel hold up and interactions between units must be known and must be viable. A study of the steady state operating characteristics of the process over all possible operating conditions will provide much of this information. Dynamic modelling does however provide valuable insight into the process that is not possible to obtain from steady state modelling. Packages have been developed that enable the dynamic response of the system to be modelled.

Dynamic simulation is classified either as a distributed system where thermal and concentration gradients are taken into account where appropriate along with time, giving a set of partial differential equations. Or the system is classified as a 'lumped' model where the thermal and concentration gradients are ignored giving a set of ordinary differential equations. The set of ODE's are less computationally expensive to use, and in most cases will give a solution that is close to the distributed model. However, in the analysis of heat integration the temperature gradients may become important and comparisons to steady state models should be made to investigate this.

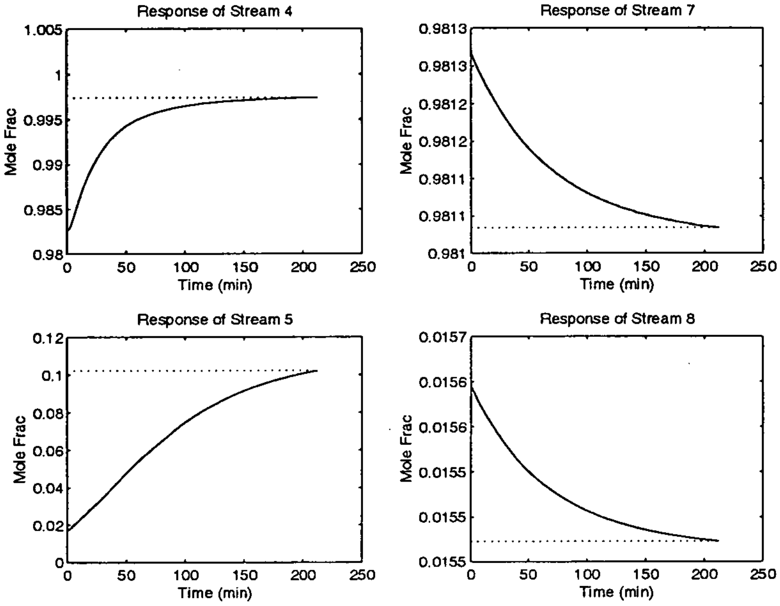
The use of a distributed model can help to identify the resilience of the system where constraints on the thermal or concentration parameters exist. For example, pinch conditions can occur between heat exchangers effecting the resilience of the system.

Hysys provides the ability to set up a system and model distillation columns dynamically [58] through the use of a lumped system. The development study was taken and placed into Hysys to compare the results of the linearised model to the dynamic simulation. However, not all of the information that is required for dynamic simulation is created at the synthesis stage of development and therefore rules of thumb governing the operating characteristics of the system have to be used.

Accepting that there is uncertainty in the design means that assessing the system using the distributed analysis can add too much analysis into the system. A far better approach is to assess the controllability of the system using a linearised approximation and then examine the resilience at specific operating points. Where possible the designer can then focus the design to accommodate these disturbances. An example of this is in the analysis of a heat integration system. The size of the heat exchangers are calculated depending upon the duty but without any accommodation made for variation of heat duties.

The distillation models assume that some controllers are present in the system. Level control in the reboiler and reflux rate are maintained along with the pressure of the vessel. The output concentration on the system is allowed to vary depending upon the feed concentration.

The two columns have been entered into the package and a step increase in the feed concentration of stream 1 is examined. The mole fraction of i-Butane is increased from 0.7 to 0.75 and the results shown in figure 4.33.



Step in Stream 1
(0.7 → 0.75 mole frac i-Butane)

Figure 4.33: Dynamic Simulation Results 1

Stream 5 and 7 correspond to $x_b(s)_{T101}$ and $x_d(s)_{T102}$ respectively in figure 4.30. Most noticeable from this analysis is that the linear model fails to predict the magnitude of interaction between the columns. The change while being in the same direction is significantly larger in the dynamic model than the linearised model. An increase in the top stream 1 leads to an increase in the mole fraction of i-Butane of stream 5 from

0.017 to 0.1 while the linear model predicts a small increase from 0.0173 to 0.01755.

With knowledge of the dynamic model the linearised approximation can be tuned to give better results. Hopefully by performing a dynamic analysis on one process alternative the linearised response of all units for all other processes can be improved.

A linearised approximation model can never be as good as a dynamic model as the effect of small interactions are neglected which can accumulate to produce a system that is difficult to control.

4.6.8 Introducing Controllers Into the System

To examine how useful a linearised system is for predicting the response of a controlled system a flash vessel can be examined with controllers being put in place. Two flash vessels are considered of different sizes of $\frac{1}{3}m^3$ and $\frac{1}{2}m^3$. Figure 4.34 shows a suitable control structure for a flash vessel where the level of the liquid is controlled by the bottom flow rate and the pressure by the top flow rate. These two controllers maintain the units operating parameters and are assumed to be present in the linearised approximation and the dynamic simulation. Control of the composition is maintained by adjusting the steam flow rate and it is desired to make an estimate of this controllability.

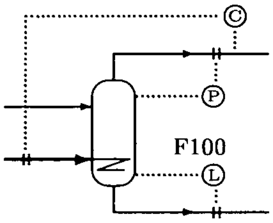


Figure 4.34: Flash Vessel Control Structure

The flash vessel is modelled in Hysys with a feed of 0.7 mole % Butane and 0.3 mole % Propane. The feed stream temperature is 48 °C and the output product purity of Butane is 0.805 mole % . It is seen likely that the controller will have to reject disturbances in the feed composition and so the effect of a step change of Butane to 0.75 mole % is analysed.

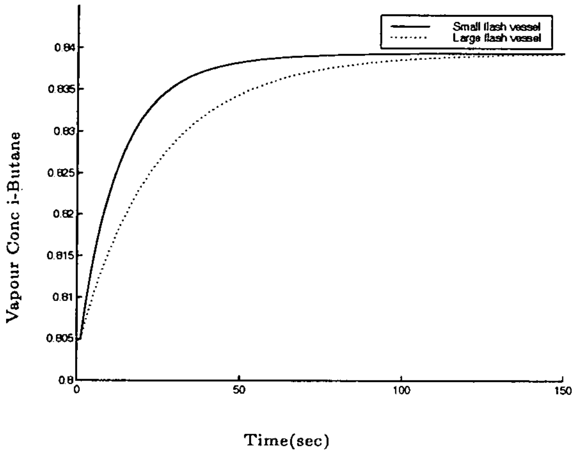


Figure 4.35: Flash System with no controllers

Figure 4.35 shows the vapour concentration of Butane of the two systems with the composition controller not present. The output concentration can be approximated by a first order response where the time constant is dependent upon the size of the vessel. As expected both systems approach the same steady state value. Larger vessels have longer response times and therefore it is expected that they will have a longer settling time with the controller in place. It could also be expected that the larger vessel will have better disturbance rejection.

Figure 4.36 shows the effect of introducing identical composition controllers into both systems to maintain product purity. The disturbance rejection of the large vessel is slightly improved with the peak of the large flash vessel being slightly less than the small vessel. However, the settling time of the system is extended. It can be expected that a linearised model of the system can give an insight into the limitations of the controller that would be used.

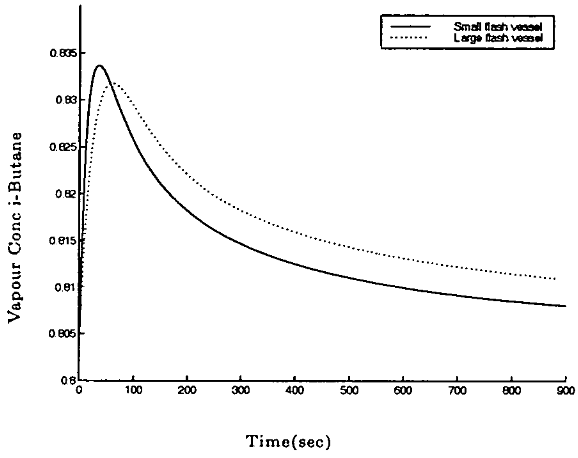


Figure 4.36: Flash system with controllers in place

4.6.9 Processes Sequencing

Efficient design is frequently obtained through the use of recycles of material or energy. These closed loops can amplify a disturbance and remove a degree of freedom making the system more difficult to control. It it therefore important to be able to analyse if any adverse effect occur and their extent in effecting the controllability of the system.

Integrated Process Distillation

A common process structure developed during synthesis is the combined process and heat integrated column. Figure 4.37 shows two process alternatives for separating three components including heat integration.

Using the linearised approximation models for the distillation columns an integrated process model can be developed. A step change in the input concentration of the middle boiling component is made and the effect examined in the output concentration of the middle stream. The graphs are shown in figure 4.38

The steady state increase for the two columns without heat integration and fixed recovery is from 88.04 % to 89.50 % . In this case the direct sequence produces a gain

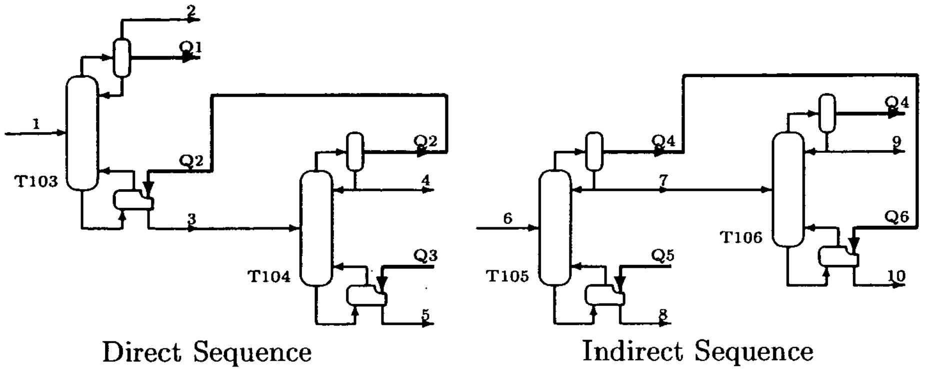


Figure 4.37: Process and heat integrated columns

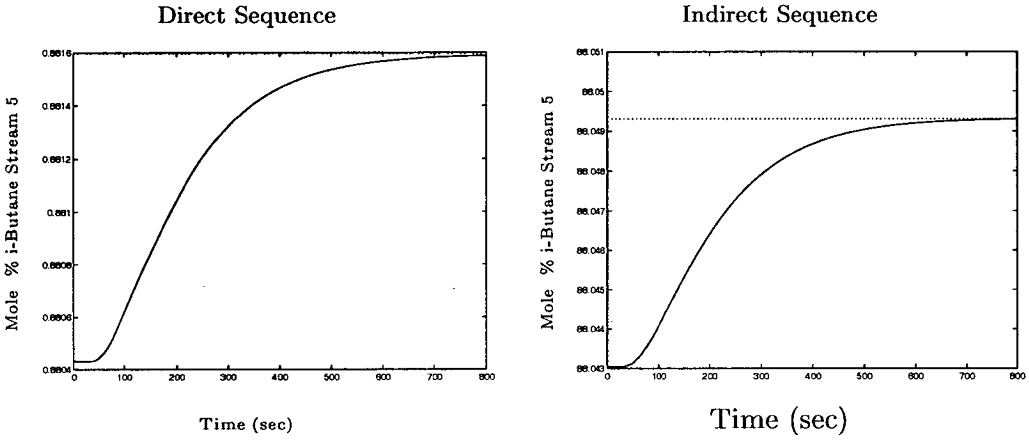


Figure 4.38: Concentration of stream 4

from 88.04 % to 88.16 % and the indirect sequence produces a gain from 88.04 % to 88.05 % . In practice the controller that will be used will attempt to maintain the system with a constant specification. It is expected in this situation that the indirect sequence would the easier process to control. The degree of variance from ideal can be measured by the two indexing methods of minimum squared error between setpoint and the output and the minimum time for closed loop system to reach steady state.

	Squared Error	Time to Steady State
Direct Sequence	$1.35 * 10^{-2}$	611 min
Indirect Sequence	$3.92 * 10^{-5}$	576 min

Table 4.13: Index Results

The indirect sequence produces a system that comes to steady state in a slightly shorter space of time than the direct sequence, along with the squared error being much smaller than the direct sequence this would indicate that this system would be easier to control for a fixed composition.

In order to analyse this system further a dynamic model of the system will have to be generated and the actual control structure can also be designed and tested.

Discussion of control methods

Different methods of analysis have different strengths and weaknesses associated with them. In order to gain an understanding of the control issues both dynamic and steady state control analysis needs to be performed. The most comprehensive analysis of the system is given by a full dynamic analysis. It enables small interactions to be analysed, however pinch conditions are neglected in the analysis as duties between units are used. A more comprehensive model could be built to incorporate the response of the heat exchangers between units. This extra level of complexity may yield little benefit, for example where the temperature of a distillation column hardly moves. This can be assessed by using the steady state resilience analysis. The linearised approximations to the column provide enough detail about the gain and the response time of the system for a review of the system to be possible, and can be improved as more understanding of the system is gained.

Steady state analysis of resilience and flexibility provide an indication as to how far the system rejects disturbances placed upon the system and how far the system can be pushed until it produces an unsatisfactory product.

None of these methods by themselves provide enough information as to how a process will react under real conditions, but together a greater understanding of the system can be achieved. Implications in the design of control structures can be obtained and the search space can be reduced by eliminating difficult to control processes .

Chapter 5

Decision Making with Multiple Objectives

The purpose of post synthesis analysis is to aid in the selection of suitable processes. The methods that have been presented help highlight the desirable features of all the processes, but a decision will then have to be made as to which process is the best. The final decision is up to the designer, but being able to formulate the results in a manner which the design engineer can interpret is important.

Most multi-objective decision making relies on the designer to formulate a weighting of the features that they would like to see in the process. These are usually weighted with respect to cost so the value of an index value is known. Then a utility function can be formulated and the decision set optimised. Multi-objective formulations can be formulated by the decision maker along two lines depending if the value function is defined or not.

- Examine the relationship between indices to see if different alternatives can be eliminated or the properties of a particular process exploited.
- Formulating the value function for each alternative and use this to evaluate the competing alternatives.

In practice some combination of the two is likely to exist. Relationship assessments are useful to reduce the search space down to a manageable size whereas formalised methods enable specific selection of the best alternative.

5.1 Relationship Assessments

A set of tools are available which do not require formal definitions of the value function to be made. Comparisons between two or more indexing results can be made to examine if a relationship exists and focus the search space down to the most applicable process.

5.1.1 Statistical Analysis

Statistical analysis can be applied to gain an understanding of the processes involved. Multivariate analysis is a well researched area where a review is given by Kendall [59]. The method considers n objects on which there is observed p variables. It is mostly used where a large quantifiable set of data exists and is used to prune down alternatives to the key decision making points. The sample space must be large otherwise relationships between tests could be missed.

An example of statistical analysis is to find the best oil from a hundred samples $(n = 100)$ from ten pieces of quantifiable data $(p = 10)$ ranging from viscosity at varying temperature points, product life time, cost etc. We are therefore want to know if the quality of one result is associated with scores in any of the other sets of results. Can the oil samples be broken down into groups of good, bad and indifferent or is the spectrum of results continuous?

Focusing upon a section of multivariate analysis called principle components analysis gives the answer to these questions. The objectives of principle component analysis is:

- To reduce the dimensionality of the problem
- Select the most useful variables

- Help visualise multidimensional data
- Identify outliers and their respective properties

Results from the analysis are placed into an observation matrix $(n * p)$ shown in equation 5.1. It is useful to consider changes around the mean value of each variable given in equation 5.2.

$$\begin{bmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{p1} & \cdots & x_{pn} \end{bmatrix} \tag{5.1}$$

$$x_{i.} = \frac{1}{n}\sum_{j=1}^{n} x_{ij} \tag{5.2}$$

In order to reduce the dimensionality of the problem each n row of the matrix can be considered as an p length vector. If a subset of dimensions p' exists which is less than p and which accounts for 75 % [1] or more of the variance then the system can be dimensionally reduced. The set of $p - p'$ can then be viewed as constituting noise to the analysis. For process systems we can assume that the designer has focused upon the most important aspects of design, dimension reduction is usually inappropriate.

The determination of linear combination of variables can be useful in determining relationships between sets of variables. To find this requires finding the eigenvalues of the covariance matrix given by equation 5.3.

$$c = \frac{1}{n} x * x' \tag{5.3}$$

x' = transpose of x

---

[1] 75 % is an arbitrary choice and the designer must judge the most appropriate value

If an eigenvalue of the covariance matrix is zero then the variance on the associated eigenvector is zero and a linear combination between the variables exists. An example of this analysis is shown for a set of oil samples. Each oil sample is adequate and has a viscosity and cost associated with it. It is therefore desirable to examine the set of samples for any additional benefit that the samples may have. For this example there are a hundred samples ($n = 100$) available[2] and for each sample the results from five tests ($p = 5$) are known (3 component compositions, viscosity and cost).

Mixture	x_1 Oil A %	x_2 Oil B %	x_3 Oil C %	x_4 Viscosity $10^{-3} Pa.s$	x_5 Cost $ /L
1	88.8	2.6	8.6	5.4	9.8
2	84.5	10.1	5.4	4.9	8.9
3	49.0	6.6	44.4	6.2	14.4
4	53.1	46.8	0.1	3.2	9.7
5	0.9	10.5	88.5	5.6	11.2
⋮	⋮	⋮	⋮	⋮	⋮

Table 5.1: Oil Viscosity Data

Using the normalised data we can get the covariance matrix from which the eigenvalues and the correlation matrix can be calculated.

	x_1	x_2	x_3	x_4	x_5
x_1	0.326	-0.280	-0.327	-0.015	-0.029
x_2	-0.280	1.272	-0.249	-0.143	0.090
x_3	-0.327	-0.249	0.601	0.095	-0.005
x_4	-0.015	-0.143	0.095	0.031	-0.007
x_5	-0.029	0.090	-0.005	-0.007	0.083

Table 5.2: Correlation Matrix

The eigenvalues show that there is one zero and therefore there must exist a linear relation among the variables. Examining the eigenvectors we get the result shown in 5.4. This shows that there is a strong relationship between x_1, x_2 and x_3. Re-examination of the original data shows that all percentages add to 100 and therefore in the analysis one percentage value can be ignored.

---

[2] Only the first five points are shown for clarity.

Eigenvalues	1	2	3	4	5
0.000	0.790	-0.033	0.030	0.587	-0.174
0.007	0.280	-0.101	-0.067	-0.099	0.947
0.076	0.546	0.099	-0.009	-0.798	-0.235
0.821	-0.001	-0.989	0.026	-0.090	-0.113
1.409	0.000	0.021	0.997	-0.029	0.070

Table 5.3: Eigenvalues and Correlation Matrix

$$(x_1\ x_2\ x_3\ x_4\ x_5)\begin{pmatrix} 0.790 \\ 0.280 \\ 0.546 \\ -0.001 \\ 0.000 \end{pmatrix} \tag{5.4}$$

Selection of data sets which best represent the task is best done by examining the eigenvalues of the correlation matrix in which with any linear variables have been removed. In the oil example with component 1 removed this then gives eigenvalues of (0.0072 0.0729 0.4803 1.1469) . From this it can be seen that cost(x_5) dominates the analysis with over 65 % of the variation. This shows that we may want to focus the analysis upon the cost implications.

If we can visualise p orthogonal axis then the familiar scatter diagram can be drawn. However, it is difficult to draw more than two axes and as a result selection of the most appropriate is essential in the analysis. Figure 5.1a shows how the percentage of component C affects the viscosity of the mixture. We expect these two to be closely related as their eigenvalues only account for a small percentage of the variation. A visual inspection of figure 5.1a shows which points are outliers. These points can be detected and either removed or analysed in detail to see if there exists a beneficial property that can be exploited. Conversely the eigenvalue for cost indicates a much greater variation, figure 5.1b shows a plot of % C present versus cost. This greater variation can be seen and a trend can not be detected.

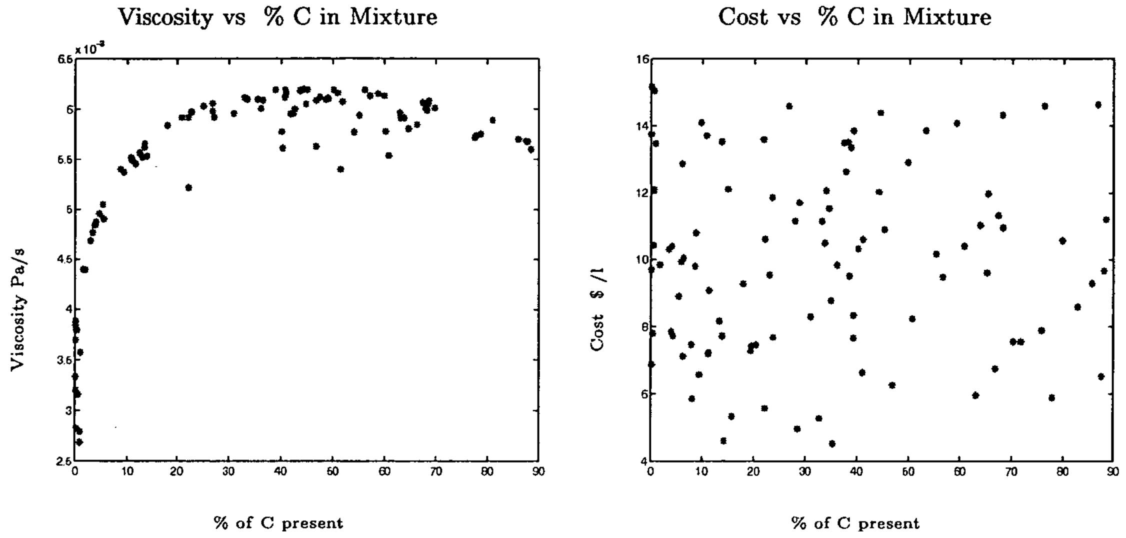


Figure 5.1: Viscosity Data Distribution

5.1.2 Dominance

Dominance is useful is determining if one sample is better than all of the other samples. It is the simplest trade off evaluation method and should be examined first. For each sample (n) there is a set of tests (p) which can be placed into an observation matrix x or as a series of p length vectors $X^1, X^2, X^3....$ where the superscript denotes the sample. $X^1 = (x_{11}, x_{12}, ...x_{1n})$ and $X_i^1 = x_{1i}$

X^1 dominates X^2 if

$$\begin{array}{rl} X_i^1 \geq X_i^2 & for\ all\ i \\ and X_i^1 > X_i^2 & for\ some\ i \end{array} \tag{5.5}$$

If X^i dominates all other X^{p-1} then all other matrices are a non-contender and the focus of analysis can be upon X^i .

5.1.3 Efficient Frontier

Alternatives which fail to make improvements in at least one rank can be eliminated from the analysis. Similar to dominance the efficient frontier considers n samples and p tests. The best way to find points on the efficient frontier is by using a process of elimination. A sample is not on the efficient frontier if it is dominated by any other sample. These samples are also known as the 'Pareto optimal set'. Figure 5.2 shows two tests θ where the efficient frontier is shown as darkened points 5.2(a) and a darkened line 5.2(b) enclosing the set of results.

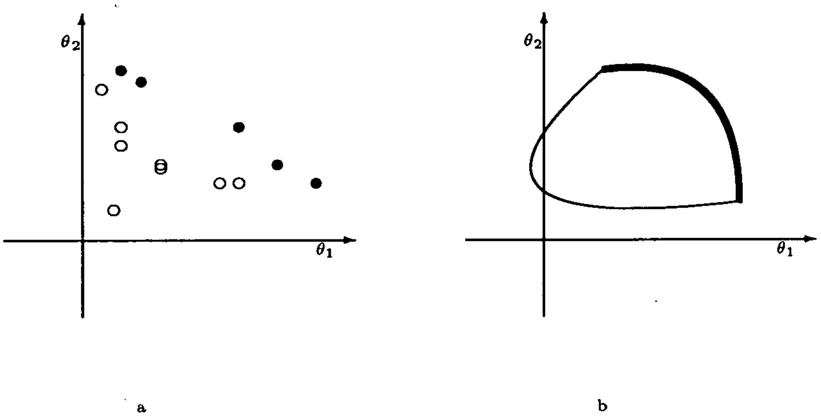


Figure 5.2: The Efficient Frontier

5.2 Value Based Assessments

When there is not an obvious best solution to a problem then assigning relative values to each of the tests applied to the samples is essential to formulating a decision. We do this all the time in everyday life in our own personal selections. A common selection is in out purchasing of products where we select the products that most suit our own lifestyle. However, we may find it difficult to explain why we chose what we did. In a design environment working with many people it is important to be able to justify a design decision. Value based assessment enables better communication and can go on to explain why we have things the way they are.

Keeney [60] has detailed a comprehensive review of the methods on value based assessments and applying the results to project planning and Cohon [61] has applied some of these techniques for programming and planning purposes.

Process	Cost	Environmental Impact	Safety	Controllability	Flexibility
1	181.34	10.82	18.29	225.88	404.54
2	186.78	11.30	18.78	230.26	387.45
3	197.66	7.90	10.27	260.97	373.21
4	208.54	14.38	22.26	267.54	307.68
5	221.23	7.98	16.59	219.30	313.38
6	266.57	15.57	17.69	223.68	284.89
7	277.45	8.45	16.28	236.84	296.29
8	279.26	14.85	23.27	256.58	333.32
9	295.58	9.17	15.26	271.93	455.82
10	301.02	15.17	24.26	280.70	350.41

Table 5.4: Process Index Results

5.2.1 Lexicographical Ordering

Lexicographical Ordering is the simplest method and probably the most widely used in practice. An example of which is alphabetical ordering where one ranking method at a time is used, and further ranking methods are only used when a draw occurs between two alternatives.

The method requires the user to rank tests in order of importance. In process design the test order importance could be Cost, Safety, Environment, Control etc. To consider samples other than the best sample from the first test a degree of uncertainty or tolerance has to be associated with the result. The extent of this tolerance is defined by the users own personal preference.

Lexicographical ordering can use either the entire set of results or the Pareto optimal set. If the entire set of solutions is used then it is possible that a non-contender object can rank equally with a dominating object but can never rank higher than it.

An example of lexicographical ordering is used to assess the results of analysis to 10 process upon which 5 tests have been performed. Table 5.4 shows the indexing data for Cost, Environmental impact, Safety Impact, Controllability and Flexibility where a low value is more desirable.

By normalising the data about the mean value the variance in results can easily be

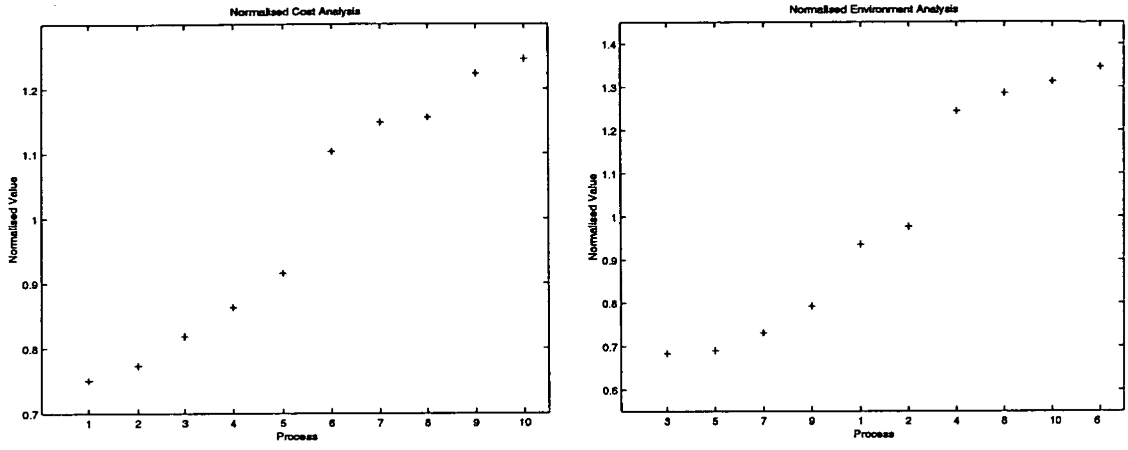


Figure 5.3: Normalised Cost and Environment Results

seen. Graphs of normalised data for each of the tests can be seen in figures 5.3, 5.4 and 5.5. These graphs can be useful in determining the degree of tolerance that should be associated with each value as distinct cut-off points are frequently visible within the data, usually caused by a dramatic change in the process structure. Where the test range can be split into distinct bands, then examining graphs of the actual data can show the cut-off points that should be used.

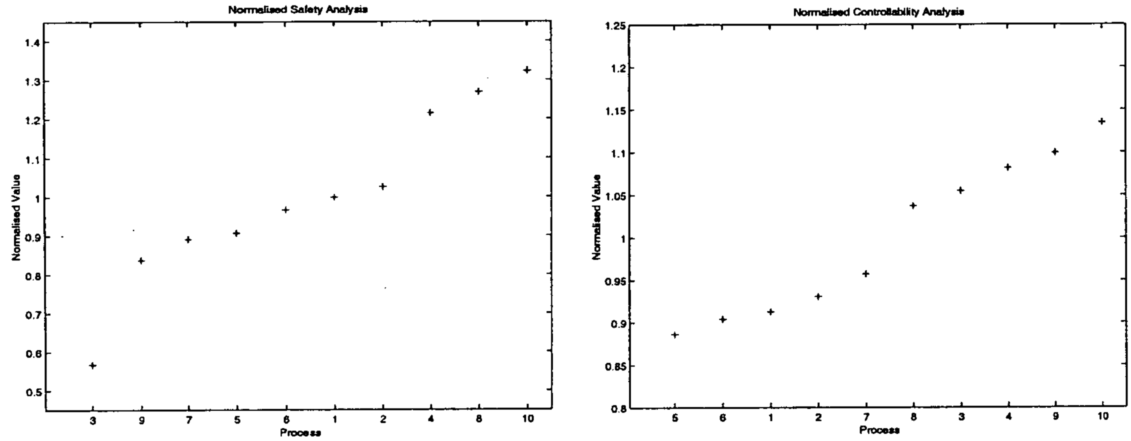


Figure 5.4: Normalised Safety and Control Results

Using the full set of data and considering the order of importance as cost, environment, safety, control and flexibility the process ranking can be achieved. From the graph of cost it can be seen that there is a gradual rise in cost from process 1 to 5, followed

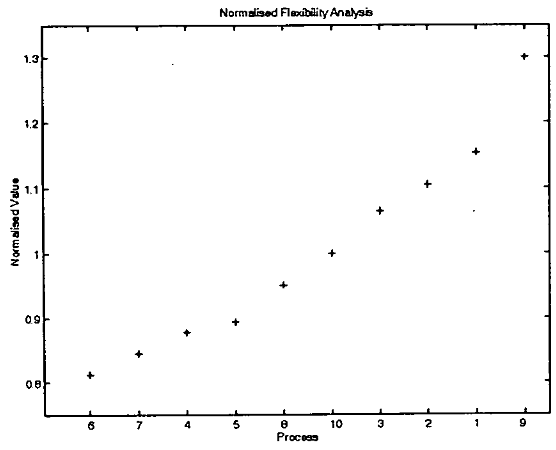


Figure 5.5: Normalised Flexibility Results

by a step increase, and again at process 8. Therefore, three sets can be considered (1,2,3,4,5),(6,7,8),(9,10), and each process with that set is considered equal.

The second sample of environment can then be employed to break each set down further. Three different groups of processes can be seen (3,5,7,9)(1,2) and (4,8,10,6). Applying this ranking to the results from the cost analysis splits the overall ranking into 7 sets being (3,5)(1,2)(4)(7)(6,8)(9)(10).

By examining the safety results a split between process 3 and 5 can be made and also process 6 and 8. This therefore separates the sets down further into (3)(5)(1,2)(4)(7)(6)(8)(9)(10). This method of analysis can continue to be applied until all tests have been examined. However, the control and flexibility analysis fail to break the subsets down any further.

This method is very dependent upon the users choice as to which criteria matter the most and where to draw the cut off point. Alternatively a a cut-off value for the tolerance can be applied to separate the processes. For example, if a strict 10 % uncertainty is applied to each of the ranking systems then a different order is obtained. Applying the same test order with this cut-off criteria the order (3)(1,2)(5)(4)(7)(6)(8)(9)(10) is obtained.

5.2.2 Indifference Curves

Indifference curves trade off one test against another to give curves of equally desirable alternatives. Given n samples, the decision maker can choose which are preferred and which are equally desirable. Then equally desirable points must lie on the same indifference curve and preferred points on a more valued curve. Figure 5.6 shows a set of indifference curves in two dimensional space.

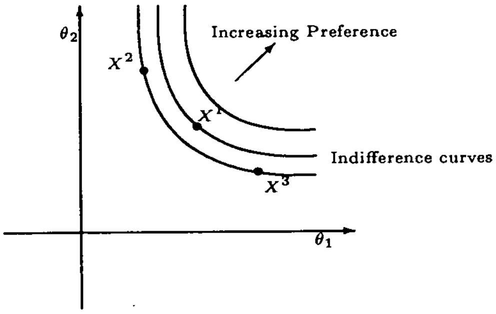


Figure 5.6: Indifference Curves

From this we can see that the decision maker does not care whether X^2 or X^3 is chosen as both provide the same amount of utility[3], but point X^1 is preferred to X^2 as it lies on a higher indifference curve.

Indifference curves can be used with the efficient frontier to formulate a maximisation problem. Figure 5.7 shows how this problem can be formulated with object X^1 being the preferred option.

As an analysis tool it is useful to ensure that the decisions being made are consistent when choosing the preferred option. Suppose the decision maker decided that X^2 is preferred to X^1 then it would be impossible to have X^3 being more preferable to X^2

.

This analysis can be expanded to n dimensional space, but becomes difficult to visualise

---

[3] Indifference curves are also referred to as utility curves

but can be described using a value function.

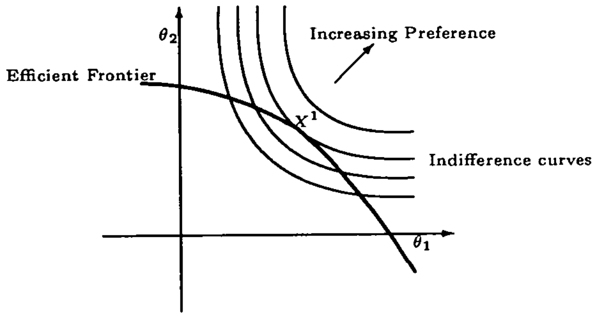


Figure 5.7: Indifference Curves and the Efficient Frontier

5.2.3 Value Functions

A function can be formulated which associates a number to each sample X^i in the evaluation space. A value function v explicitly defines the indifference cure and can easily be expanded to n dimensional space. A typical value function for 2 dimensions is shown in equation 5.6.

$$v(X^i) = c_1 * X_1^i + c_2 * X_2^i \quad where\ c_1\ and\ c_2 > 0 \tag{5.6}$$

Value functions require determining explicitly the trade off between variables and is useful in reducing the problem down to a single figure. If a value function can be formulated then the problem can be reduced to an optimisation problem. A common method is to reduce everything down to a cost value function. By carefully utilising past accounting figures a cost for many indexing methods can be obtained.

5.3 Decision Methods Applied to Process Systems Analysis

The combination of methods applied to post synthesis analysis enables decisions about the process structure to be made. Statistical analysis most useful when analysing a large set of data. If there are a large number of processes available with lots of tests being carried out upon those processes then focusing down upon the important tests and their effect can dramatically reduce the search time. In process design a principle concern is the search for the outlying process, the processes that do not conform to the rules and see if there are any beneficial properties that can be extracted from it.

Dominance and the efficient frontier are useful methods to try and exclude processes where a much better alternative exists. It does not make sense to look at processes that fail to improve in at least one index and if the process excels in all indices then no further analysis needs to be taken.

It is unlikely that these tools will be unable to reduce the search space down to the most desirable solution and a value trade off will have to be carried out. Lexicographical ordering and Indifference curves break the problem down into manageable pieces but require a lot of user interface with the results of each test.

If the user has a very good understanding of the value trade offs then a value function can be formulated and an optimisation tool applied. In certain areas a lot of work has been carried out to reduce the problem to a common value. For example, insurance concerns have turned safety analysis into producing risk assessment and return a liability cost. However, areas such as controllability, flexibility and environmental analysis are much harder to quantify and the value judgements between people can vary enormously.

Multiple Objective decision making requires balance and good judgement. These tools only help a designer achieve balance the judgement is down to the user.

Chapter 6

Hydrogen Cyanide Case Study

This Case study demonstrates the use of the post process synthesis techniques on a case study for the manufacture of hydrogen cyanide (HCN). The problem specification is to produce 20,000 tonnes of HCN per year from an eqimolar ammonia/methane feed. The method of synthesis for this case study is by using the CHiPS package [23].

The main reaction to produce HCN without air being present.

$$NH_3 + CH_4 \leftrightarrow HCN + 3H_2 \quad +251\ KJ/mol$$

This reaction takes place at temperatures of 1200-1300 °C . We also have a secondary reaction taking place decomposing the ammonia.

$$2NH_3 \leftrightarrow N_2 + 3H_2$$

The overall consumption of ammonia is greater than 90 mol% with about 1/20 being consumed by the second reaction. According to Kirk and Othmer [62] the output stream from the reactor contains the following.

20	mol%	hydrogen cyanide
70	mol%	hydrogen

3	mol%	ammonia
1	mol%	methane
1	mol%	nitrogen

H_2SO_4 and SO_2 have to be added to the product to act as a stabiliser to prevent polymerisation of the HCN.

The HCN case study provides an interesting plant in terms of safety, controllability and environmental aspects. HCN is a hazardous material due to its toxicity and its ability to spontaneously polymerise. Therefore, when developing a plant design inherent safety is of great interest. There is also the problem that vast amounts of hydrogen are produced, not only is hydrogen an extremely flammable material but it also has the ability to cause hydrogen embrittlement of the plant equipment. Other important aspects of the plant that post process synthesis should address are the problems of formation of by-products and the problems caused by the large temperature differences occurring across the plant. Not only does this allow for interesting heat integration, but it also affects the controllability, operability and flexibility of the plant. It is hoped that the post process synthesis analysis will quantify some of these problems.

6.1 CHiPS Synthesis

Some assumptions about the HCN process have to be made for a CHiPS synthesis run to take place. Initially the ammonia decomposition reaction was ignored. Because the production of nitrogen will not affect any of our product streams it was assumed that we could accept quite high concentrations in the hydrogen/methane stream as this will be used as fuel. However running the process without the production of the nitrogen failed to produce the diversity of process structures expected with only one feasible structure being returned. Therefore the nitrogen production would have to be introduced giving more opportunity to increase the range of possible design alternatives.

In order to simplify the analysis in this preliminary case study a fixed conversion reactor, with a number of potential conversions will be used. The system can be allowed to produce other products apart from the principal product and the fuel product.

6.1.1 Allowable Units

For synthesis to be carried out the allowable units that can be used must be defined. The chosen units and their applicability to the problem determines the size of the search space that will have to be examined.

Reactor

The basic reactor model available in CHiPS can only deal with one reaction. This requires that both the hydrogen cyanide reaction and the ammonia decomposition reaction are incorporated within the same stoichiometry. In order to do this a reactor model in Aspen was used to formulate an approximation to the reaction conditions. At reaction conditions of 1300K, 90% of ammonia is converted into hydrogen, and a further 5% is decomposed into nitrogen and hydrogen. However, we also want to check how this is affected by the change in the input concentration. With these conversions the following approximation to the stoichiometry of reaction can be made.

$$1.1NH_3 + CH_4 \leftrightarrow HCN + 3.15H_2 + 0.05N2$$

Using this stoichometery enables the reaction products to be estimated and allows a set of structures can then be produced. These structures can then be reexamined to see if the reactors output accurate. If the differences prove to be large then a new run will have to be carried out.

Separation

With the separation section of the analysis there are two options which examine either the possibility of running with different recoveries in one column or introduce the use of multiple columns. This analysis to looks into the possibility of running with 1 column set to a top and bottom recovery of 96%. With the high concentration of hydrogen and methane being present, it is unlikely to be economical to run the synthesis with a distillation train only and therefore a flash separation is also be allowed.

6.1.2 Allowable Products

CHiPS requires that we define which products can be produced. In the preliminary design we will allow only two products to be produced.[1] The selection of suitable products is important as it governs the feasibility of the synthesis stage.

Hydrogen Cyanide Product

The principal product of hydrogen cyanide must have a purity greater than 98 mol%, and has to have a flow greater than 10 kmol per hour. The principal contaminant will be ammonia which has to be in a concentration less than 1 mol%.

---

[1] These also can be refined at a later date

Fuel Product

Any hydrogen produced can be used as fuel, assuming that this will go to a burner also acceptable are high concentrations of methane, and reasonable concentrations of nitrogen. However in order to keep NO_x emissions low ammonia and hydrogen cyanide are not permissible in this stream, therefore the following specification upon this stream can be made. A fuel stream that has a mole fraction of hydrogen greater than 60 mol% and methane greater than 10 mol% is acceptable. This should also ensure that the synthesis package does not flash the feed stream and specify the methane fraction as a product. Also to ensure that the design is carried out and that the feed stream is not designated a product stream it is also stipulated that the fuel stream must contain nitrogen in a concentration greater than 1 mol%. The two major contaminants of ammonia and methane must be in concentrations less than 5 mol%.

6.1.3 Costing basis

The costs for the streams needs to be known, and the following costing parameters are used by the synthesis package.

NH_3	4	$ /Kmole
HCN	32	$ /Kmole
CH_4	1	$ /Kmole
Fuel Gas	0.3	$ /Kmole

6.1.4 Synthesis

A `task` object is generated with the unit descriptions and the allowable products. The `task` object is then inputed in to the CHiPS package for synthesis. The 10 best solutions are then taken and analysed.

Early on in the design it can be seen that some of the designs out of the returned processes are not feasible. For example processes that try to distill the hydrogen/methane stream will not be built in practice due to the low temperatures or high pressures required.

Eliminating the infeasible structures, we end up with the following processes, that can be taken forward for further analysis.

6.1.5 HCN Process 1

Process 1 is the process that would most likely be designed if the Douglas [3] hierarchy is followed through. The reactor product is quickly cooled and the hydrogen and methane removed through a flash drum. The product purity of hydrogen cyanide is obtained through the use of a distillation column with a ammonia vapour recycle being passed back to the reactor with about 15 mole % of the recycle gas containing hydrogen cyanide.

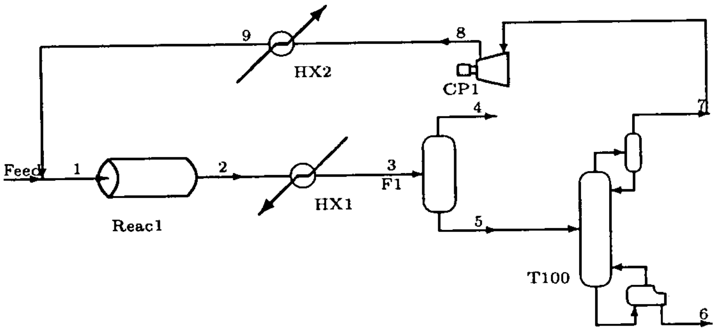


Figure 6.1: HCN Process 1

	Feed	1	2	3	4	5	6	7	8	9
Vapour Fraction	1.00	1.00	1.00	0.817	1.00	0.00	0.00	1.00	1.00	1.00
Temp (C)	300	300	550	7.98	2.41	2.41	76.2	29.5	70.6	259
Pressure (KPa)	900	900	900	900	600	600	600	600	908	907
Molar Flow (Kgmole/h)	200.0	206.0	396.6	396.6	299.8	96.9	90.8	6.0	6.0	6.0
Mole Frac (Ammonia)	0.500	0.505	0.010	0.010	0.000	0.042	0.001	0.662	0.662	0.662
Mole Frac (Methane)	0.500	0.486	0.024	0.024	0.031	0.002	0.000	0.031	0.031	0.031
Mole Frac (HCN)	0.000	0.009	0.233	0.233	0.000	0.956	0.999	0.307	0.307	0.307
Mole Frac (Hydrogen)	0.000	0.000	0.721	0.721	0.954	0.000	0.000	0.000	0.000	0.000
Mole Frac (Nitrogen)	0.000	0.000	0.011	0.011	0.015	0.000	0.000	0.000	0.000	0.000

Table 6.1: Process 1 Stream Flows

6.1.6 HCN Process 2

This is the strangest of all of the processes being considered and not one that would usually be generated under the Douglas hierarchy. The feed is mixed with a recycle and the hydrogen cyanide separated. In practice it would be expected to see this separation as silly, but part of the purpose of post process synthesis is to separate out some of the ridiculous ideas from the feasible set of solutions so that a design engineer can focus their attention upon realistic processes. This process hasn't been eliminated early on because all of the process temperatures are feasible.

One of the main difficulties is separating the hydrogen cyanide from a predominantly hydrogen stream. By adding in ammonia the reflux temperature is brought down to a more attainable temperature. Also if the ammonia is stored as liquid and the feed to the reactor has to be gaseous then utilising this difference in enthalpy could prove to be effective. Start up, shut down and control could be problematic with the feed to the reactor being dependent upon the recycle. A pump which handles a liquid recycle of ammonia and hydrogen cyanide may eliminate this plant on safety reasons.

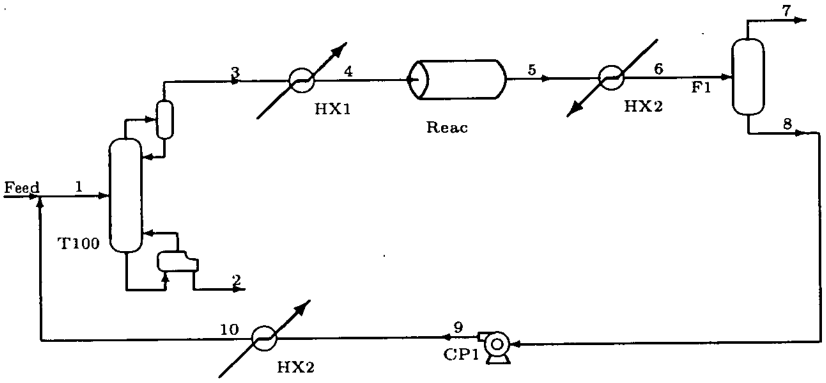


Figure 6.2: HCN Process 2

6.1.7 HCN Process 3

This process is the indirect sequence with the hydrogen cyanide being removed first after the reaction sequence. The hydrogen and excess methane is removed in a flash

	Feed	1	2	3	4	5	6	7	8	9	10
Vapour Fraction	0.99	0.79	0.00	1.00	1.00	1.00	0.858	1.00	0.00	0.00	0.51
Temp (C)	0.01	0.01	92.9	0.25	300.6	550	21.9	14.8	14.8	14.8	94.0
Pressure (KPa)	900	900	900	900	900	900	900	600	600	900	900
Molar Flow (Kgmole/h)	200.0	295.0	90.9	204.1	204.1	392.9	392.9	297.8	95.0	95.0	95.0
Mole Frac (Ammonia)	0.500	0.353	0.011	0.505	0.505	0.010	0.010	0.000	0.042	0.042	0.042
Mole Frac (Methane)	0.500	0.340	0.000	0.491	0.491	0.026	0.026	0.034	0.002	0.002	0.002
Mole Frac (HCN)	0.000	0.308	0.989	0.005	0.005	0.231	0.231	0.000	0.955	0.955	0.955
Mole Frac (Hydrogen)	0.000	0.000	0.000	0.062	0.062	0.721	0.721	0.951	0.000	0.000	0.000
Mole Frac (Nitrogen)	0.000	0.000	0.000	0.000	0.000	0.011	0.011	0.015	0.000	0.000	0.000

Table 6.2: Process 2 Stream Flows

vessel with a liquid recycle of ammonia present. It is expected that this process would have a lower risk factor, but the benefits may be offset by higher cooling duties required. The distillation sequence that is used is equivalent to a single distillation column with a partial condenser and a liquid and vapour distillate stream. This process may also produce an interesting controllability problem as the cooling duty on the distillation column will be difficult to achieve and maintain. This process has the lowest loss of hydrogen cyanide and ammonia to fuel gas compared to the other processes. A large proportion of HCN is recycled back to the reactor system which on further analysis may significantly reduce selectivity.

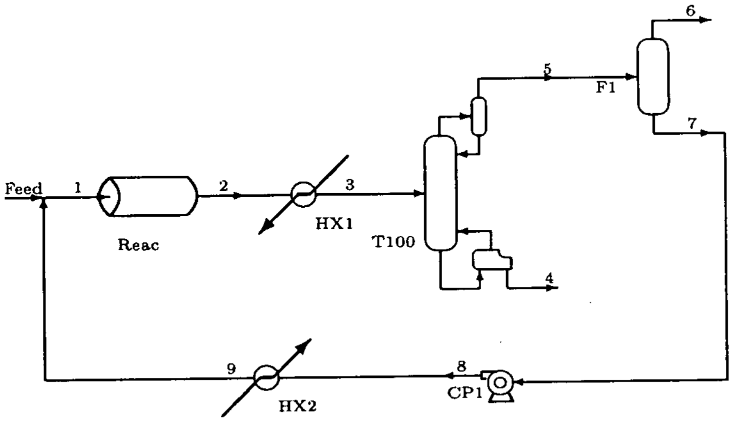


Figure 6.3: HCN Process 3

	Feed	1	2	3	4	5	6	7	8	9
Vapour Fraction	1.00	1.00	1.00	0.870	0.00	1.00	1.00	0.00	0.00	1.00
Temp (C)	300	300	550	25.7	94.7	-5	-11.5	-11.5	-11.5	300
Pressure (KPa)	900	900	900	900	900	900	600	600	900	900
Molar Flow (Kgmole/h)	200.0	206.0	396.6	396.6	90.8	305.8	299.8	6.0	6.0	6.0
Mole Frac (Ammonia)	0.500	0.505	0.010	0.010	0.001	0.013	0.000	0.662	0.662	0.662
Mole Frac (Methane)	0.500	0.486	0.024	0.024	0.000	0.031	0.031	0.031	0.031	0.031
Mole Frac (HCN)	0.000	0.009	0.233	0.233	0.999	0.006	0.000	0.307	0.307	0.307
Mole Frac (Hydrogen)	0.000	0.000	0.721	0.721	0.000	0.935	0.954	0.000	0.000	0.000
Mole Frac (Nitrogen)	0.000	0.000	0.011	0.011	0.000	0.015	0.015	0.000	0.000	0.000

Table 6.3: Process 3 Stream Flows

6.2 Process Ranking

Each conceptual design has a degree of uncertainty associated with it. Costing is only an indication as to the profitability of each process. Each process has their own strengths and weaknesses and assessing these will give a much better understanding of the processes.

6.2.1 Costing

The preliminary cost index for the process costing is shown in table 6.4.

Process	Profit per year million $
1	20.8
2	17.0
3	9.4

Table 6.4: Synthesis Costing

From the synthesis costing it would be easy to assume that process 1 should be the process of choice and the other processes disregarded. A difference of $ 3 million could be a justification to only explore process 1 further, however errors in the costing analysis need to be examined and the true economic value of each process explored. These costings can be placed into the revised costing spreadsheet which gives further information about the profitability of each plant. The revised costing shows the net present values and internal rates of return for each process and the results are shown in table 6.5.

Process	NPV at 10 % Million $	IRR %	Pay-back years
1	122.4	99.4	0.01
2	99.5	99.3	0.01
3	54.9	98.7	0.01

Table 6.5: Updated Costing

These figures in themselves are strong evidence that the costing assumptions that are being used have some serious flaws associated with them. While it might be possible to accept that a net present value of 1 $ 22 million may be possible an IRR close to 100 % and a pay-back time of 0.01 years is suspicious and would indicate that a miscalculation with the capital cost is likely to have occurred.

The capital cost for each process is about $ 118,000, with most of the expense of the plant being consumed in operating costs. By recalculating the data in a spreadsheet allows the cost functions to be examined for errors which can then be corrected.

Reactor System

The capital cost of the reactor is evaluated using a simplified equation 6.1 from Guthrie [26].

$$\textit{Capital Cost}\ (\$) = 1917 * D^{1.066} \tag{6.1}$$

D=Reactor Diameter (m)

This assumes that the reactor is a simple plug flow reaction vessel and makes now allowance for packing or heating requirements placed upon the system. In the production of hydrogen cyanide a process furnace would be used, with the cost being governed by the duty associated with it. Therefore, a more appropriate formula would be.

$$\textit{Capital Cost}\ (\$) = \frac{M\&S}{280}(17.5 * 10^{3}) * Q^{0.85} \tag{6.2}$$

Q = absorbed duty GJ/hr

Unfortunately, the synthesis model does not evaluate the heating duty required in the process furnace, therefore post calculation has to be done. The average heat capacity

Process	Heat Duty GJ/hr	Revised Furnace Cost $	Fuel Cost $	Original Reactor Cost $
1	27.6	1,113,723	1,173,000	83,850
2	27.4	1,106,859	1,164,500	82,258
3	27.5	1,110,292	1,168,750	83,850

Table 6.6: Revised Furnace Cost

of the stream throughout the furnace is evaluated using a thermophysical property calculation and with the heat of reaction known the costing of the column can be evaluated. The revised cost of the furnace evaluates to be $ 302,000 for process 1 down to $ 301,000 for process 2.

This results in a overall change in the profitability of each plant, however the differences in capital cost between plants is negligible and does not effect the ordering of the plant choice by economics. These also appear to be exceptionally low prices for the furnace and upon closer examination it was found that the default Marshall and Swift index of 288 is too low to account for modern prices, instead a more appropriate figure would be 1062.

The synthesis package also does not calculate the running costs of the furnace. The duty required is known and calculation of the cost of heating can be made, assuming that the cost of heating is 4 $ /GJ and the efficiency of the furnace is 80%.

These corrections shown in table 6.6 can be entered back into the spreadsheet which has a significant effect upon the capital and operating costs. Also the cause of these errors can be corrected in the `reaction module` so that further synthesis can be carried out without the same errors occurring.

Distillation System

The capital cost for the distillation system is evaluated using the following equations 6.3 6.4 and 6.5 from Guthrie [26].

$$Capital\ Cost\ (\$) = (1 + 0.0147 * (P - 3.4))\left(\frac{4.23 * M\&S}{288} * 7620 * D * \left(\frac{H}{12.2}\right)^{0.68}\right) \tag{6.3}$$

$$Tray\ Cost\ (\$) = 0.61.S.\frac{M\&S}{280} * 111.41 * \left(\frac{D}{1.22}\right)^{1.9} \tag{6.4}$$

$$Intrument\ Cost\ (\$) = 4,000 \tag{6.5}$$

Again a change in the Marshall and swift index is also required in the analysis of the system. The distillation cost equations can be improved to incorporate the pressure and the design materials that will have to be used. It is suggested that the second set of equations 6.6 6.7 and 6.8 also from Guthrie [26] is used instead. The heating and cooling requirements of the column can also be updated to present prices.

$$Capital\ Cost\ (\$) = \left(\frac{M\&S}{280}\right) * 5771.8^{1.066} * H^{0.802} \tag{6.6}$$

$$Tray\ Cost\ (\$) = \left(\frac{M\&S}{280}\right) * 75.7 * S * D^{1.55} \tag{6.7}$$

$$Instrument\ Cost\ (\$) = 15,000 \tag{6.8}$$

Process	Original Separator Cost $	Revised Separator Cost $
1	27,082	112,761
2	28,889	118,462
3	27,863	113,255

Table 6.7: Revised Separation Costing

The alterations to the costing structure have given further insight into the costing of the plant and the updated costing of the processes is shown in table 6.8.

Because large changes to the costings have been introduced into the system the designer could either rerun the synthesis package with the modifications present or accept the design structures present and develop them further. Because each of the designs still demonstrate a potential profit and changing the cost function is unlikely to produce any further structures this analysis focuses upon the three designs already developed.

Process	NPV at 10 % Million $	IRR %	Pay-back years
1	17.9	72.5	0.38
2	15.1	69.3	0.44
3	10.6	62.1	0.61

Table 6.8: Revised Costing

6.2.2 Fire and Explosion Hazard Ranking

The fire and explosion index can be applied to the class of process with revised costings to give the results shown in table 6.9. The material factors for the components present are shown in appendix D.1.

Process	Fire and Explosion Index	Damage Factor	Maximum Damage $
1	7.4	1.95	3,100,000
2	7.9	1.96	2,800,000
3	7.3	1.85	3,000,000

Table 6.9: Fire and Explosion Index

The analysis returns a similar index for each of the designs, with process 2 having the highest index, where the large ammonia-methane recycle making makes a significant contribution. Process 2 suffers from a higher index for the distillation column because of the higher operating temperature, but does benefit from a lower damage factor because of the addition of ammonia, therefore resulting in a lower maximum probable damage.

This creates the situation where the fire and explosion index indicates that the ranking of the processes should be 3,1,2. If the priority is to assess the potential damage caused should an accident occur then the processes should be ranked 2,3,1. This means that deciding which plant is the most inherently safe is a choice that is dependent upon the design criteria and hence has to be left to the designer.

Too much detail can be read into the fire and explosion index giving the impression that either process 3 or 2 is the inherently safer plant. This method has not included compressors and heat exchangers and other ancillary equipment which would be required.

This post synthesis method does return information about each unit so that potential benefits to the system can be examined. The fire and explosion results for each unit are shown in appendix D.2. From these results the following conclusions about the safety of the plant can be obtained.

- The mixer in process 2 processing HCN increases the Fire and Explosion index.
- The addition of ammonia in process 2 reduces the maximum potential damage.
- The safety of the reactor system is consistent regardless of which process is used.

6.2.3 Chemical Exposure Ranking

The chemical exposure index returns information about each stream and its potential hazard, the user must evaluate this potential hazard with respect to the inventory being carried. The chemical exposure index demonstrates some of the problems of returning a single index for the whole process. The index relates to specific streams where a worse case scenario on the amount of loss which could occur is used. The hazard can be reduced by reducing the inventory of hazardous materials present which is determined at the detailed design stage. Selected streams from the flowsheet are used and the indices returned are shown in appendix D.3.

This post synthesis method highlights the large discrepancies in the safety of the product stream, which is important as the inventory of each product stream is likely to be similar. Process 2 produces HCN at a high temperature and pressure, this has a high probability of producing an aerosol effect and hence contribute to the 10 Km hazard distance. There is little difference is streams leaving the reactor and so further analysis can concentrate upon the safety of the distillation system. Process 1 has the lowest index across all of the streams and we could therefore consider it to be the most inherently safe with process 2 being the least safe.

6.2.4 Environmental Evaluation

The environmental index has been set to examine the global warming potential of each stream present and return an overall index for the plant with the substitution/elimination index.

Process	Feed GWP	Product GWP	Flue GWP	Substitution/Elimination index
1	7.5	3.22	0.59	0.183
2	7.5	7.48	0.59	0.079
3	7.5	2.24	1.16	0.514

Table 6.10: Global Warming Potential

The substitution/elimination index is only used as an indicator as to which process may be the best. Improvements to the process can only be made by either substituting a waste stream, or eliminating a waste stream and making it into a useful product, therefore the lower the index the better. This would indicate that process 2 was the most desirable with a lowest index. This is because of the high index of the product stream which contains the highest molar flow of ammonia and only just makes the necessary product specifications. In this case it would be sensible only to look at the life cycle assessment which ranks the processes as 3,1,2.

6.2.5 Flexibility

A flexibility index Matlab file is generated for each process. Possible disturbances to the system are disturbances to the feed composition, recovery in the distillation column and disturbances in the extent of reaction. If we take each of these disturbance in turn and identify any potential problems with each system.

Disturbing The Feed Composition

Perturbations to the feed are made with an ideal variation being 1% of the molar flow of each component. The results of these perturbations are shown in table 6.11.

All of the process are bounded by an upper limit of the ammonia feed and a lower limit on the methane feed. The resulting flexibility index for each process is similar with process 2 having a slightly lower index than the other two processes. However, the model is based on a linear approximation of the system and a fixed conversion in the reactor is used, therefore care must be taken when examining such a small difference in the indices.

Because each process is being bounded by the higher concentration of ammonia, the system is being constrained by the hydrogen cyanide specification. Analysis of the distillation system and the recovery should give us greater information as to the flexibility of the system.

	Flexibility index	Ammonia feed bound	Methane feed bound
Process 1	0.342	100.34	99.66
Process 2	0.304	100.30	99.69
Process 3	0.352	100.35	99.65

Table 6.11: Feed Composition Flexibility

Disturbing the Distillation Recovery

To test the flexibility of the distillation column perturbations to the recovery of the key components are made, with an ideal variation being 1 % of the original value. The results are shown in table 6.12, and show that process 2 suffers from poor flexibility around the distillation column. This is probably due to the larger quantity of material that the distillation column has to process. Therefore, if there is any degradation in the control structure on process number 2 then the system would fail to produce an on specification product.

	Flexibility index	Tops recovery bound	Bottoms recovery bound
Process 1	2.10	1.0000	0.0196
Process 2	0.30	0.9830	0.0200
Process 3	2.06	1.0000	0.0196

Table 6.12: Distillation Recovery Flexibility

Disturbing the extent of reaction

Disturbances in the conversion in the reactor, will show how sensitive the system is to uncertainty in the reaction products. The original extent of reaction for each component is shown in table 6.13. The result of disturbing the extent of each component by 1% is shown in table 6.14. Process 2 has the lowest flexibility index, and any uncertainty we have with the reaction would affect process 2 the most. Process 3 has the highest flexibility, which is due to the placement of the distillation column straight after the reactor vessel.

	H_2	N_2	CH_4	NH_4	HCN
Process 1	285.38	4.53	-90.60	-99.66	90.60
Process 2	279.78	4.44	-88.82	-97.70	88.82
Process 3	285.36	4.52	-90.59	-99.65	90.59

Table 6.13: Original Extent of Reaction

	Flexibility index	H_2	N_2	CH_4	NH_4	HCN
Process 1	0.344	286.36	4.51	-90.28	-99.32	90.29
Process 2	0.305	280.63	4.43	-88.55	-97.40	88.55
Process 3	0.353	286.36	4.51	-90.27	-99.30	90.27

Table 6.14: Extent of Reaction Flexibility

6.2.6 Controllability

A Matlab control file can be generated for each process, a general model for each unit is formulated from knowledge of the steady state operating conditions[2] and the size of the unit. These can then be linked together using the topology information. In order to gain information about the entire process modelling the response of each unit with respect to each component would be necessary. Because the HCN product is constrained by the ammonia concentration and because the NO_x emissions in the fuel gas is also dependent upon the ammonia concentration, attention should therefore focus upon the amount of ammonia present.

---

[2] Models are formulated in HYSYS and perturbations from normal operating conditions introduced. These gains are used in the formation of the linear model.

6.2.7 Linearised Control Models

Identifying potential disturbances and their affect upon the system is critical to the synthesis of a control system. A disturbance has the potential to propagate through the system , producing a system that is difficult to control. A disturbance can also manifest itself into other disturbances upon the system and examination of this interaction can be essential in determining the feasibility of a process.

Potential disturbances to a unit are identified and their affect upon the output modelled using a Laplace transform. This greatly reduces the effort required to solve linear differential equations and enables the output of units to be dependent upon multiple inputs. The response of the fuel and hydrogen cyanide products from each systems are examined by disturbing the feed composition to the system. The method to find a transfer function plus time delay is detailed by Seborg [63].

Reactor model

The main interest in the output of the reactor is the ammonia concentration. An increase of 1 % in the input concentration of ammonia will lead to an output increase of approximately 1 % . The reactor output temperature will also affect the down stream processing and therefore will have to be considered. The same increase in the ammonia concentration results in a 10 % drop in the outlet temperature. The calculated the gain in the system and an estimated settling time of 1 minute is used to formulate a linearised model. Also assuming a 5 minute time delay for any disturbance to propagate through the reactor is also included in the model which is represented using a second order pade approximation. The model is expressed in terms of transfer functions and the result of combining these functions is shown in figure 6.4.

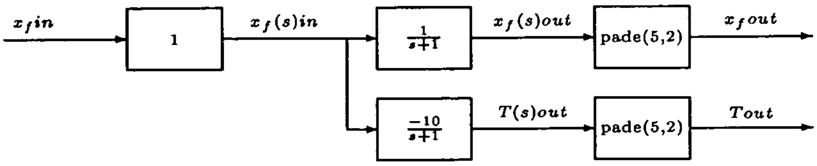


Figure 6.4: Linearised Reaction Model

Flash model

The output of the flash vessel is dependent upon temperature, feed concentration and pressure. It has been assumed that pressure remains constant. The large temperature variations generated by the reactor cannot be ignored and therefore temperature variations have been considered in the model. Examining a steady state model reveals that a 1 % increase in the ammonia concentration leads to an increase of 0.5 % in the top and the bottom concentration, the change has no significant impact upon the output temperatures. Changes in the input temperature have a significant effect upon the output from the flash vessel. An increase of 1 °C leads to a reduction of 0.08 % in the top concentration and an increase of 0.02 % in the bottom concentration. The temperatures of the outputs have a gain of unity with respect to changes in the feed temperature. The system is assumed to settle after 1 minute for both product streams and an estimate of 1 minute time delay for the disturbance to propagate through the flash drum is also included. The transfer function model is shown in figure 6.5.

Distillation model

A similar linearised model was developed for the distillation, with the output dependent upon the input concentration and composition. The dynamic behaviour of the distillation column can be evaluated either by examining the steady state model or applying the dynamic equations as given by Wahl [57]. By using the Wahl equations the distillation model can be made to fit different distillation column sizes, reflux rates and feed compositions. A short cut can be made if all of the columns are similar by examining the response of one column under steady state conditions and applying the time gains afterwards. Steady state modelling reveals that a 1 % increase in the input

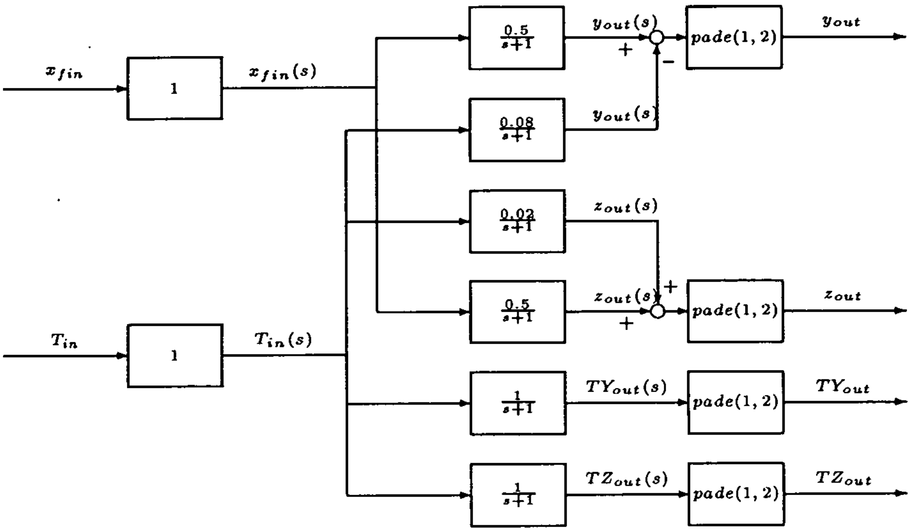


Figure 6.5: Linearised Flash Model

concentration leads to an increase of 1.1 % in the top products and a 1.8 % increase in the bottoms. A 1 °C increase in the feed temperature leads to a 1.5 % decrease in the top concentration and a 2.2 % increase in the bottom concentration. It can also be estimated that the time delay will take 5 minutes to appear in the top products and 1 minute for the bottoms. From this the linear transfer model can be obtained which is shown in figure 6.6.

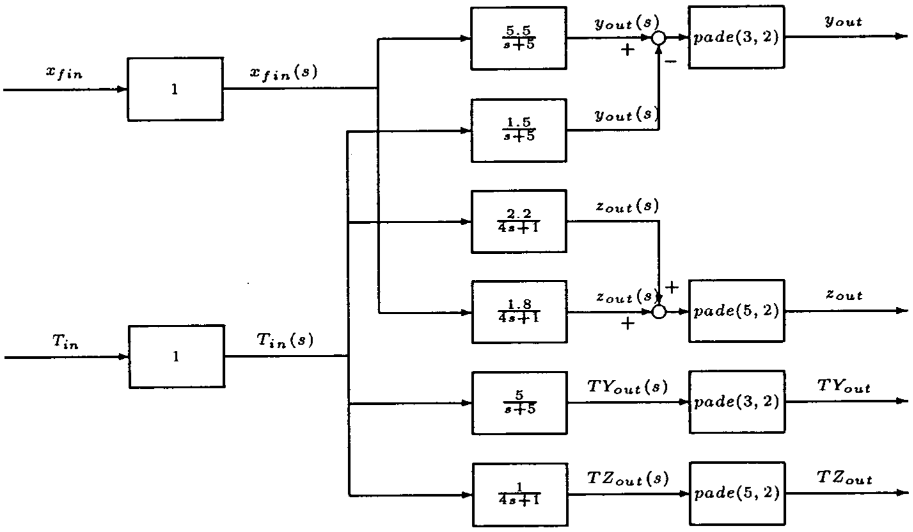


Figure 6.6: Linearised Distillation Model

A step impulse to the system is introduced to the ammonia concentration and the disturbance recorded. The results of this disturbance for the output from the flash drum are shown in figure 6.7, and the distillation column is shown in figure 6.8. The initial sinusoidal response is caused by the pade approximation to the time delay.

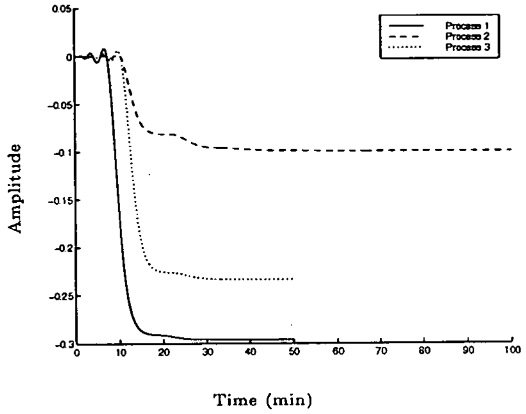


Figure 6.7: Flash drum output

Table 6.15 contains the results of the step impulse. Process 1 produces an amplitude which is three times greater than process 2. The response time of the system is dependent upon the location of the flash drum. Process 1 has a flash drum closest to the feed and hence the smallest response time. Process 2 and 3 both have an extra distillation column between the feed and the distillation column and hence have a longer and almost identical response time.

The maximum amplitude of the output is small at 0.3, which indicates that controlling the output of any of the processes should not be a significant problem. Process 1 has a concentration of ammonia of 3 mol% in the fuel gas and a constraint of 5 mol% this would mean that the feed concentration of ammonia could increase by 6 mol% before the system becomes unfeasible. Therefore, the systems should be able to reject any disturbance in the feed ammonia concentration. There is no inverse response in the system and the effect of a recycle is just visible with a second smaller decline in the concentration after 30 minutes.

Of greater interest is the output from the distillation column. The flexibility index has

	Final Value	Settle Time	Rise Time
Process 1	-0.30	16.6	5.2
Process 2	-0.10	39.0	15.9
Process 3	-0.23	25.3	5.5

Table 6.15: Flash drum output results

proved that maintaining the specification on the hydrogen cyanide product is a critical problem, and any overshoot or inverse response may signal a process that could prove difficult to control. The results of the step disturbance on the ammonia concentration in the HCN product are shown in figure 6.8, and the numerical results are shown in table 6.16. The graph clearly shows that process 2 has the best disturbance rejection of all the processes, and also has the longest settling time and rise time. This is not consistent with the flexibility index which would indicate that process 2 was the least flexible, and therefore the least capable of rejecting disturbance. However, the flexibility index does not include the effect of temperature upon the system. In order to fully understand the controllability of each process a complete heat integrated system will have to be analysed [3]. The disturbance filters through much quicker with process 1 and 3. The constraints on the hydrogen cyanide stream are much tighter than the fuel stream and control is a more important issue.

With a mole fraction of ammonia of 0.5% process 2 can reject disturbances in the feed up to 0.3% of the original value while process 3 can only reject disturbances of 0.1% in the ammonia concentration. The long settling time in process 2 may also prove to be advantageous as control of the distillation column would probably involve utilising the reflux and hence the cryogenic cooling requirements of the system.

	Final Value	Settle Time	Rise Time
Process 1	2.76	22.1	5.33
Process 2	1.65	31.9	14.8
Process 3	3.90	25.6	4.67

Table 6.16: Distillation output results

Using the two measures of controllability of minimum squared error between the set

---

[3] See section 6.2.9

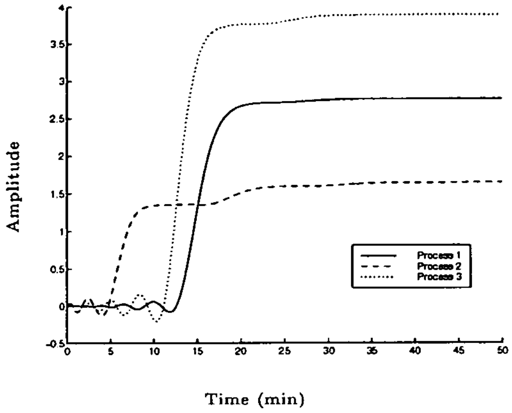


Figure 6.8: Distillation column output

point and the output and the time to steady state the differences in controllability of the processes can be evaluated and are shown in table 6.17. From this it can be seen that process 2 could be considered to be the most controllable as the disturbance propagation is small.

	Flash Vessel Output		Distillation Output	
	Squared Error	Settle Time	Squared Error	Settle Time
Process 1	0.09	16.6	7.6	22.1
Process 2	0.01	39.0	2.7	31.9
Process 3	0.05	25.3	15.2	25.6

Table 6.17: Controllability Index Results

Disturbance rejection can also be shown by the introduction of an impulse to the system. An impulse to the system highlights the effect of the rise time, and demonstrates how the impulse will travel through the system. The concentration of ammonia from the flash vessel and the distillation column are shown shown in figure 6.9 and numerical results are shown in table 6.18.

	Peak Time	Settle Time
Process 1	5.9	13.4
Process 2	9.1	14.5
Process 3	9.1	16.2

Flash Drum Output

	Peak Time	Settle Time
Process 1	14.5	21.8
Process 2	5.65	22.9
Process 3	12.6	28.8

Distillation Output

Table 6.18: Impulse Numerical Results

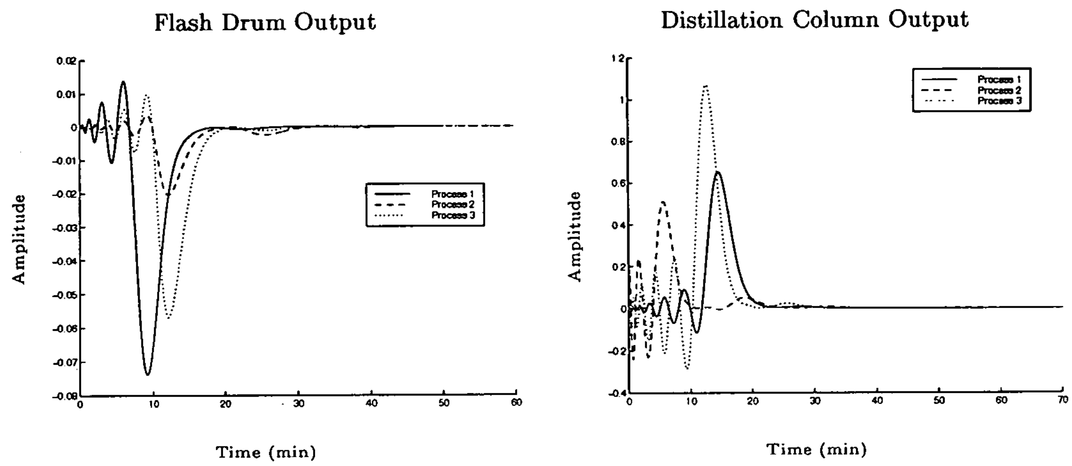


Figure 6.9: Impulse Results

6.2.8 Dynamic Control Models

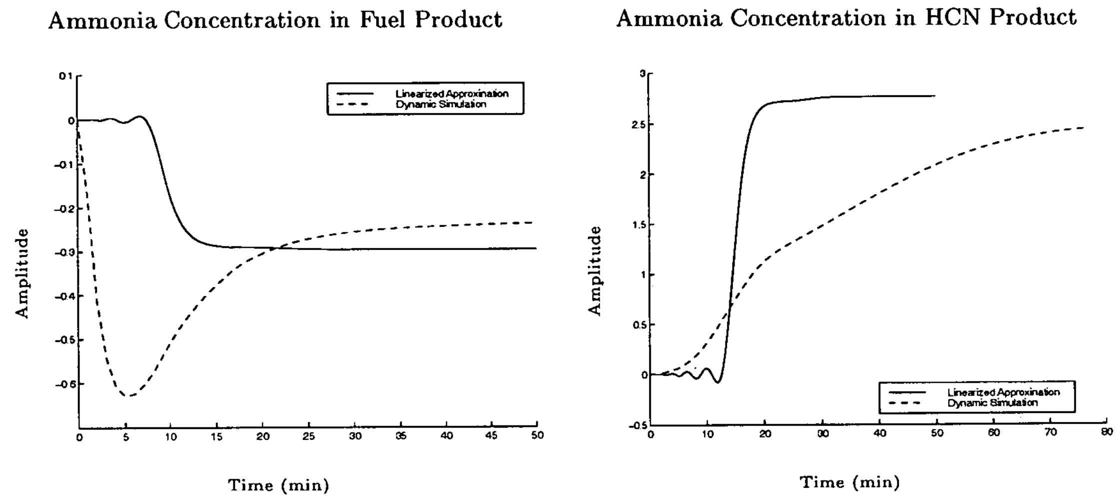
The linearised models can only give an approximation to the system. Each model is evaluated to operate for a small disturbance. If the disturbance propagates throughout the system, then the linear model is likely to fail and incorrect conclusions could result. Therefore a dynamic simulation of each process to assess the linear models needs to be carried out.

Each process has been modelled in HYSYS, and a dynamic simulation carried out with an increase of 0.5 mol% of the ammonia concentration in the feed. The results for each process are shown in figures 6.10, 6.11 and 6.12. These processes are modelled without heat integration.

Process 1

Figure 6.10 shows the comparison between the linearised approximation results and the dynamic simulation. The fuel product from process 1 demonstrates a large peak response, before settling down to the steady state value at about 20 minutes. This peak is not shown in the linearised approximation and is probably due to the influence of the output temperature from the reactor, which influences the flash vessel quickly while the time taken for the ammonia concentration is much slower. The linearised model could be improved by changing the settling time and response time for the temperature influence.

The ammonia concentration in the dynamic simulation in the HCN product has a much slower rise time, but both models still approach the same steady state value. Likewise the linear model can be improved by increasing the rise time coefficient in the model.


Ammonia Concentration in Fuel Product

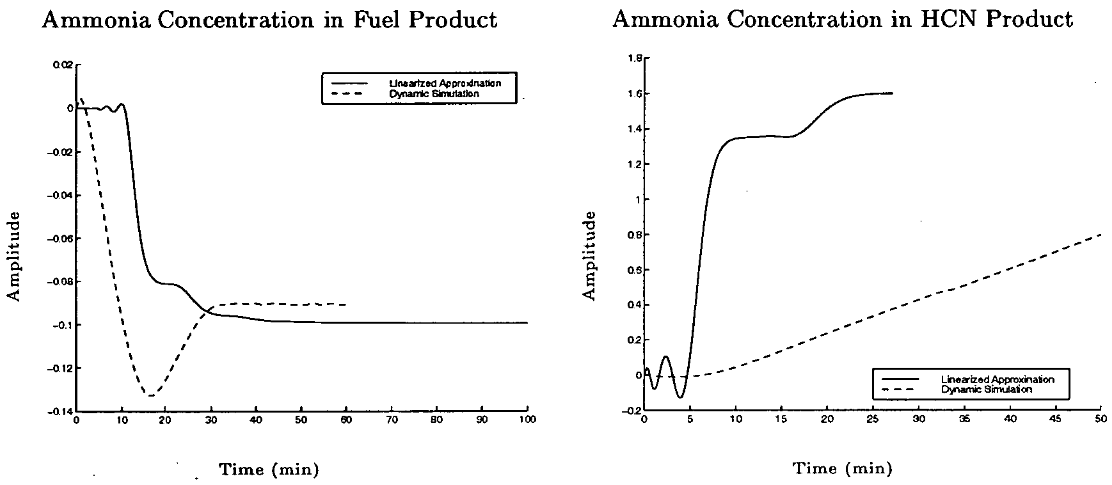
Ammonia Concentration in HCN Product

Figure 6.10: Response of Process 1

Process 2

A main discrepancy between the linearised model and the dynamic simulation is shown by process 2 is shown in figure in figure 6.11. The linearised model predicts very short rise time for the ammonia concentration in the HCN product stream and a secondary disturbance caused by the recycle. The dynamic simulation is different and shows a very long rise time. The linear model used assumed that each distillation column is similar, but the distillation column in process 2 is different as a large ammonia reflux is present. To improve the model a larger rise time for the distillation column would have to be incorporated.

The disturbance has no problem in propagating through the top of the column and onto the flash vessel where the two modelling methods produce similar results. The peak response in the flash vessel is again present in the dynamic model and not shown by the linearised approximation.


Ammonia Concentration in Fuel Product

Ammonia Concentration in HCN Product

Figure 6.11: Response of Process 2

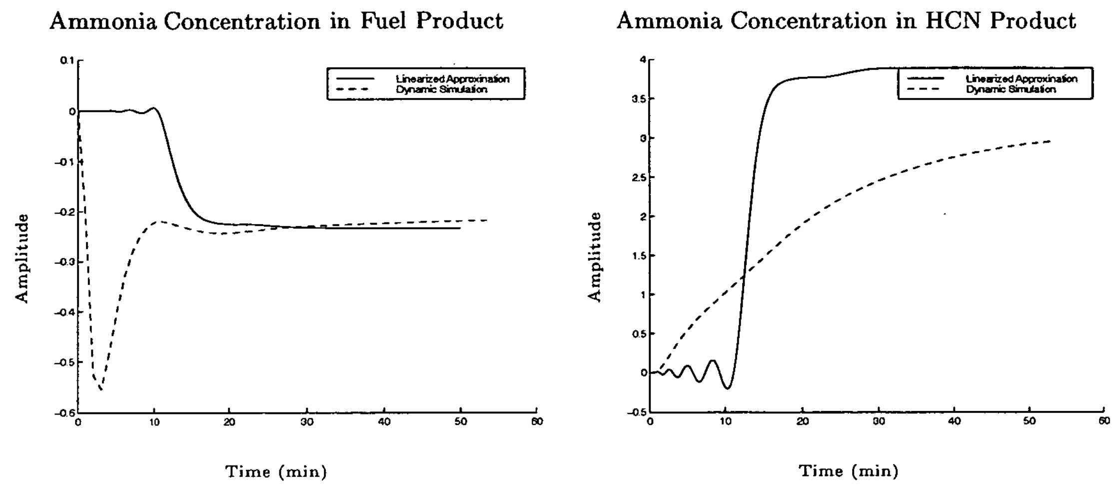
Process 3

The results from comparing the two modelling methods is shown in figure 6.12. Process 3 structure is similar to Process 1 and hence demonstrates a similar response. The peak response from the fuel product is sharper than process 1 due to the removal of HCN prior to the flash vessel. The same improvements to the linear model as process 1 can be made, by increasing the rise time in the distillation column and reducing the response time of the flash vessel to changes in temperature.

To understand the response of the system the linear model has to be refined against a dynamic simulation or the user must have detailed knowledge of the units involved.

6.2.9 Integrated Influence

Disturbance rejection gives information about the systems ability to reject perturbations to the system, but the analysis ignores heat interactions between units. Heat


Ammonia Concentration in Fuel Product

Ammonia Concentration in HCN Product

Figure 6.12: Response of Process 3

integration can dramatically effect the viability of a system as more heat exchangers are required in order to maintain the system at a suitable operating point. Analysis of the integrated influence between units will also allow the design engineer to assess problems with start up and shut down of the process.

In order to do this we need to know the heat integration of the process. In this case only the reactor outlet stream can be heat integrated with the recycle heater and the distillation reboiler. The heat integration for each process is shown in figures 6.13, 6.14 and 6.15.

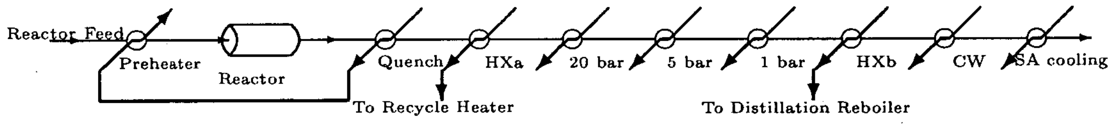


Figure 6.13: Process 1 Heat Exchangers

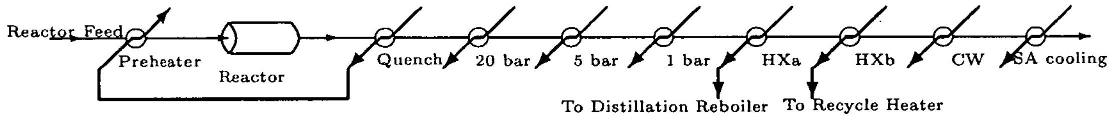


Figure 6.14: Process 2 Heat Exchangers

As has been demonstrated the linearised approximation methods can be applied, however the complexity of introducing a heat integrated distillation system results in a system

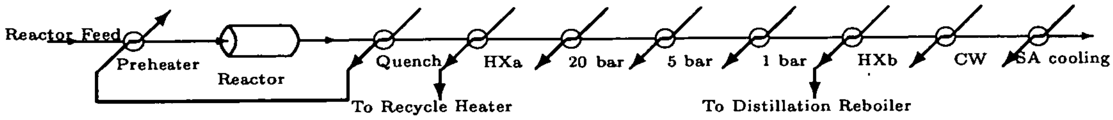


Figure 6.15: Process 3 Heat Exchangers

that is difficult to set up and understand. With more recycles being introduced a greater margin of error between the Dynamic and Linearised model occurs. A far better approach is to generate a dynamic model of the system which has been done using HYSYS. The heat integrated models can then be compared to the models that have not been heat integrated.

Process 1

The result of the heat integration compared to the non-heat integrated case is shown in figure 6.16. The trend is similar for both the Fuel and the HCN product. The HCN output is the main point of interest as during heat integration the loss of a degree of freedom in the distillation column may determine how controllable this process is. A slightly lower amplitude is seen with the heat integration case. This is due to the fact that the reboiler duty is now fixed. As the concentration is increased a larger reflux is required in order to maintain the product specification. The reboiler temperature decreases leading to a larger vapour flow in the column. The reflux ratio is perfectly controlled therefore the vapour products and the reflux rate increase. This results that heat integrating this system should have an increase in controllability.

Process 2

The heat integrated case for process 2 is similar to process without heat integration as shown in figure 6.17. There is only a small divergence from the ammonia concentration in the product in both instances. The mixing effect of recycling and then separating results in a process that is insensitive to disturbances in the feed. The disturbance in the fuel product with heat integration is small at 0.3, but it is twice as large as

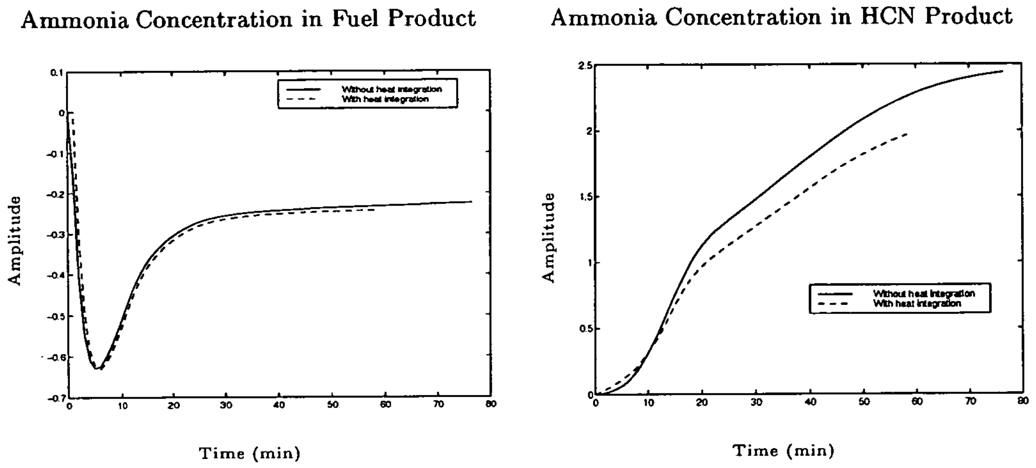


Figure 6.16: Dynamic Response of Process 1

compared to the process without heat integration.

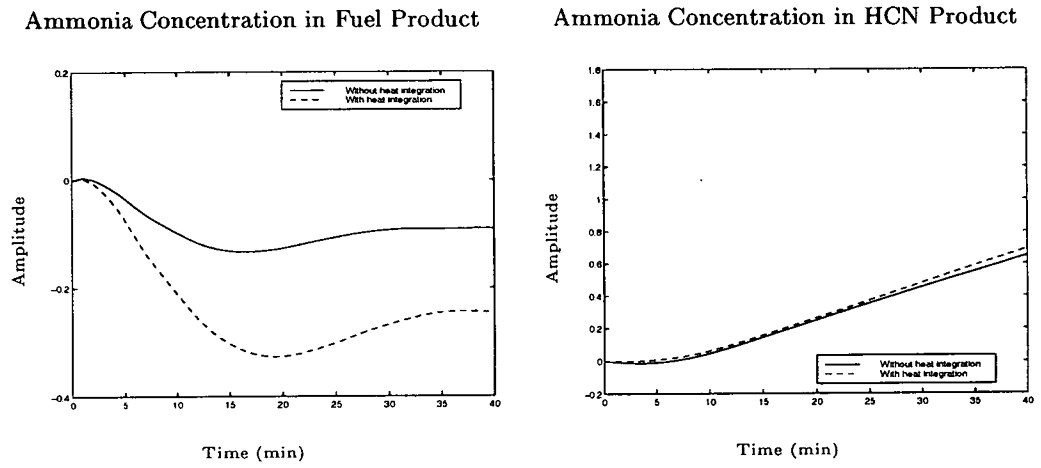
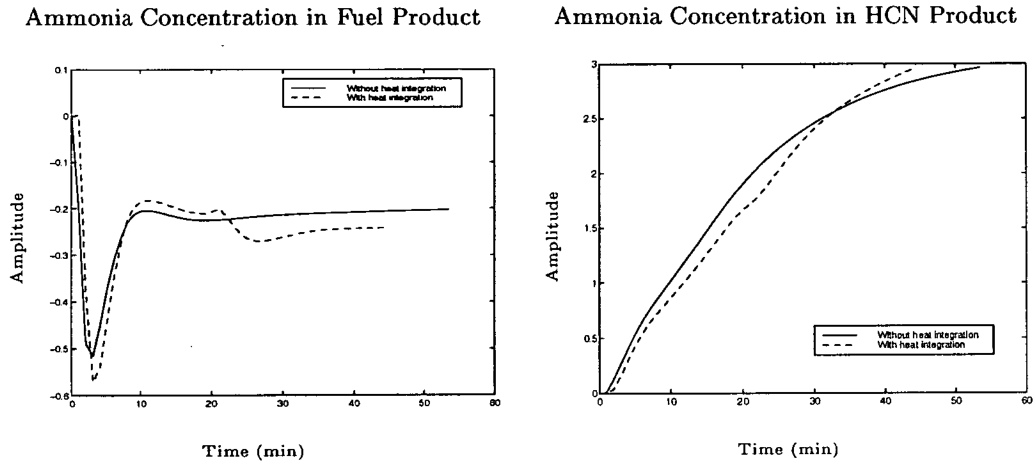


Figure 6.17: Dynamic Response of Process 2

Process 3

The heat integrated and non-integrated results for process 3 are shown in figure 6.18. The trend is similar for the ammonia concentration in both product streams. The final ammonia concentration in the HCN product approaches a slightly higher value than the non-heat integrated system. This is probably due to a lower temperature stream entering the distillation column resulting in less loss from the top of the column.

Process 3 shows that heat integration can disturb the transition from operating states. In particular a number of small deviations from the process without heat integration can be seen in the fuel product.


Ammonia Concentration in Fuel Product

Ammonia Concentration in HCN Product

Figure 6.18: Dynamic Response of Process 3

By comparing the processes with heat integration and and those without it can be seen that there is generally only a small deviations exist for the main disturbances of interest. Therefore, the analysis into controllability can focus upon the processes without heat integration and the analysis of the linearised model to the dynamic model is applicable.

6.3 HCN Study Discussion

In the HCN case study we have developed three processes with different characteristics. Our analysis has shown the need to be able to update and correct initial synthesis costing. Obtaining one process which is affordable, maximises safety, minimises environmental impact and is controllable is impossible as each criteria favours a different process. Also the way of examining a criteria can determine which process is most favourable. Cost shows that Process 1 is the most favourable process with a net present value $ 7 million more than Process 3. Examining safety reveals that Process 2 has a favourable damage factor associated with it but the chemical exposure potential of the process is very large. The environmental evaluation would favour Process 1 and 3 and the controllability analysis favours Process 2.

	Process 1	Process 2	Process 3
Net Present Value. ($)	17.9	15.1	10.6
Internal Rate of Return. (%)	72.5	69.3	62.1
Fire and Explosion Index.	7.4	7.9	7.3
Damage Factor.	1.95	1.96	1.85
Maximum Damage. (million $)	3.1	2.8	3.0
Product Stream Exposure Hazard Distance.(m)	137	10,000	19.8
Total Chemical Exposure index.	30.13	269.71	31.39
Total Global Warming Potential.	3.81	8.07	3.4
GWP substitution/elimination.	0.183	0.079	0.514
Flexibility of Feed Composition.	0.342	0.304	0.352
Flexibility of Distillation Recovery.	2.10	0.30	2.06
Controllability, Squared Error of Flash Vessel.	0.09	0.01	0.05
Controllability, Settle Time of Flash Vessel.	16.6	39.0	25.3
Controllability, Squared Error of Distillation Column.	7.6	2.7	15.2
Controllability, Settle Time of Distillation Column.	22.1	31.9	25.6

Table 6.19: Case Study Result Summary

Table 6.19 shows a summary of the indexing results. Because each process excels in at least one of the tests the three processes developed can be considered to be a part of the Pareto optimal set. With three process alternatives available the most appropriate decision making tools are lexicographical ordering and indifference curves.

If the designer specifies that the order of importance of indexing methods is cost, safety, environment and control with a 20 % tolerance upon the results then lexicographical ordering can be applied. This means that on a cost basis process 1 and 2 would then rank equally followed by process 3 as an inferior process. The safety indices would then have to be applied to separate process 1 and 2 further. The fire and explosion index does not differentiate significantly between the two processes, but the chemical exposure index is definite in ranking process 1 better than process 2. Further indexing methods would not be required to assess the final ranking of the processes. If it was felt by the designer that the difference in and further index between processes was significant then that index should either have more significance and be moved further up the order list or the prior indexing methods tolerance should be increased.

Obtaining a meaningful indifference curve requires good financial data from previous designs or the designer to be exact in their trade off values. With this information the problem can then be reduced down to a cost basis. Because previous financial data does not exist further analysis needs to be carried out and the designs developed. Once this is done the extra protection measures that have to be employed can be costed and the value function evaluated.

Chapter 7

Ethylene Case Study

The ethylene ($H_2C = CH_2$) case study applies the techniques of post synthesis analysis to the production of a plant capable of producing ethylene. Ethylene is an important chemical due to the reactivity of the double bond, creating a basic building block for an entire branch of organic chemistry. Ethylene is used in the production of polystyrene, polyvinyl chloride and polyethylene. It is a flammable gas and exhibits near ideal thermo-physical properties. The production of ethylene requires processes with a large number of units and has a great range of operating temperatures.

There are various methods for producing ethylene, with a main production method being thermal decomposition or cracking of ethane. Thermal decomposition is the process of adding heat to break chemical bonds in a substance which is an efficient and relatively inexpensive process. The method and manufacturing techniques are well documented; and kinetic and thermodynamic data is readily available. Most of the design decision differences occur in the separation section and this analysis will focus upon the design alternatives.

7.1 Design Brief

The design of the ethylene plant is to produce 12,000 tonnes of ethylene a year. Ethylene is produced by the thermal cracking of ethane to ethylene, the chemistry of the reaction is given by Froment [64] and is summarised by.

$$C_2H_6 \leftrightarrow C_2H_4 + H_2$$

Secondary reactions also occur to form acetylene and methane.

$$C_2H_4 \leftrightarrow C_2H_2 + 2H_2$$
$$C_2H_6 + H_2 \leftrightarrow 2CH_4$$

In order to prevent coke build up within the reactor the conversion of ethane is kept low. Economic studies have revealed that the removal of hydrogen is essential before distillation of the product can occur. Therefore, the study will focus upon the purification of the methane, ethane, ethylene acetylene and propane components to produce desirable products or recycle reactants. The yield of ethylene depends upon the total pressure and concentration of ethane being fed to the reactor. After the removal of hydrogen a typical process contains the following concentration of components as given by Kirk and Othmer [65].

Methane	0.1 %
Ethane	51.0 %
Ethylene	39.7 %
Acetylene	5.3 %
Propane	3.9 %

7.2 Synthesis Method

7.2.1 Allowable Units

Three units will be allowed in the synthesis stage. Two distillation columns one with a partial condenser and one without and a reactor capable of converting the acetylene to ethylene.

- Distillation Columns

  Partial Condenser

  The synthesis engine is capable of utilising a high specification distillation column with a top and bottom products recoveries at 99%, the column also has a partial condenser. We are likely to find that this column will only be suitable for the removal of light ends, but post synthesis analysis should highlight the viability of this option.

  Total Condenser

  It is expected that low specification separations will utilise a total condenser. Therefore, a total condensing column is made available to the synthesis engine with a recovery of 96%.

- Acetylene Reactor

  Acetylene is a highly explosive component and has little market value, and therefore it is desirable to remove the acetylene before it reaches high concentrations that may prove to be hazardous. Therefore the synthesis engine has to have the ability to introduce a hydrogenation reactor to convert the acetylene back to ethylene.

  $$C_2H_2 + H_2 \leftrightarrow C_2H_4$$

  Hydrogen can be added directly before the reactor and the conversion of acetylene is 98 % and all of the hydrogen is consumed. Excess hydrogen is undesirable as the reaction will continue and produce ethane.

7.2.2 Allowable Products

Three products are allowed to be produced in the synthesis stage.

- Principle Ethylene Product

  The principle product of ethylene from the system has to be in a concentration greater than 98 mol%. Any flow level of this product is accepted, so the system is not prevented from continuously refining low specification streams.

- Low Specification Ethylene Product

  We will also allow a low specification ethylene product to drawn from the process providing that the flow is kept small. In effect this stream will be a converted acetylene stream and a concentration greater than 88 mol% is specified. In order to ensure that only the small converted acetylene stream is used a second specification that the flow must be less than 6 kmol/hr is imposed.

- Recycle Stream

  The synthesis stage is concentrating on the separation sequence and ignores any recycles. Therefore, the recycle stream will have to be taken off as a product and integrated into the flowsheet at a later point. The constraints on the recycle are that ethane must have a concentration greater than 90 mol% and to prevent splitting streams too far a specification that the stream must have a flow greater than 10 kmol/hr is also imposed. In order to prevent build up of heavy oils the concentration of propane is also limited to 1%.

- C3+

  The heavier components need a release from the system and a stream containing propane and above is accepted as a product. A low specification product as it can be used as fuel therefore a mole frac greater than 80% is specified. A specification of 80% is chosen to prevent loosing product to the fuel stream.

7.2.3 Costing

Synthesis is carried out on the basis of cost, without recycles being present the synthesis of the separation system will produce similar streams. Attention is therefore focused upon the capital and operating cost of each process, and not upon the value of the product streams, the cost function used are given by Guthrie [26].

7.2.4 Synthesis Results

The synthesis stage returns results which are shown in figures 7.2 and 7.3 and the flowrates are shown in appendix E.4. The results are returned in order of preliminary cost, with the cheapest being process 1. For each process the ethylene product is removed first with the rest of the system recovering the low specification products. Design differences occur with the placement of the hydrogenation reactor and the sequence of separation of the low specification products. The costing data does not reveal any significant differences between each of the processes. Further costing will have to be carried out to find out how much of this cost is consumed by the capital and operating costs and how sensitive the profit is to each of these.

Process 1	328000 $
Process 2	334000 $
Process 3	339000 $
Process 4	341000 $
Process 5	342000 $
Process 6	344000 $
Process 7	354000 $
Process 8	392000 $
Process 9	396000 $
Process 10	408000 $

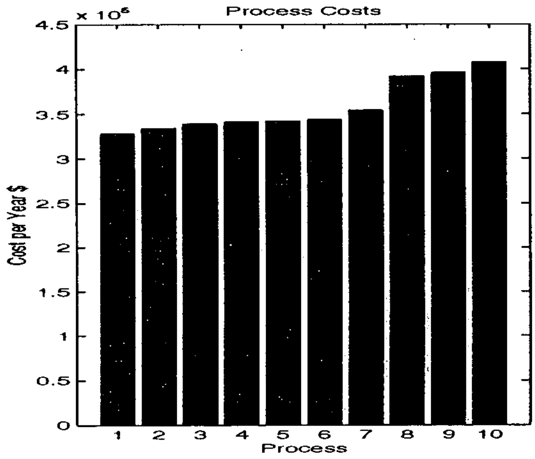
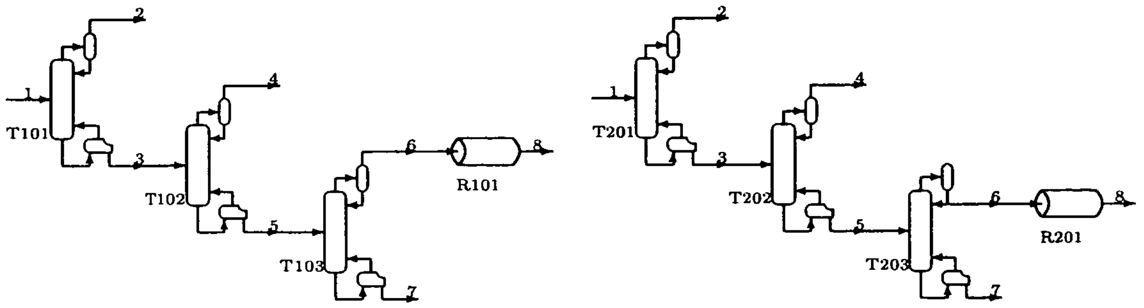


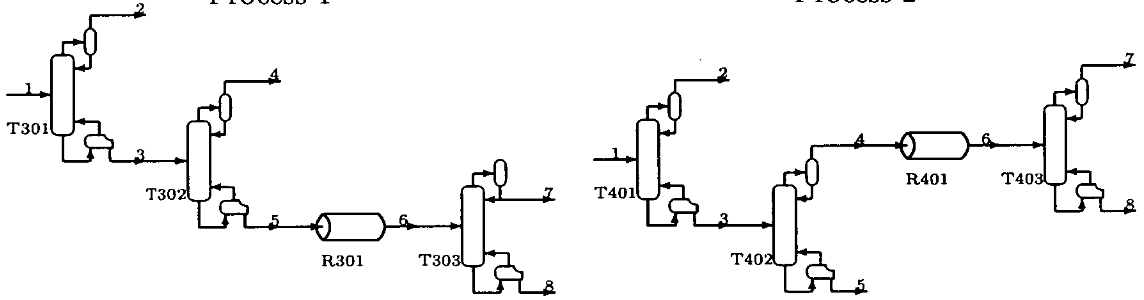
Figure 7.1: Synthesis Costing

Process 1 and process 2 both have a similar structure with the hydrogenation reactor



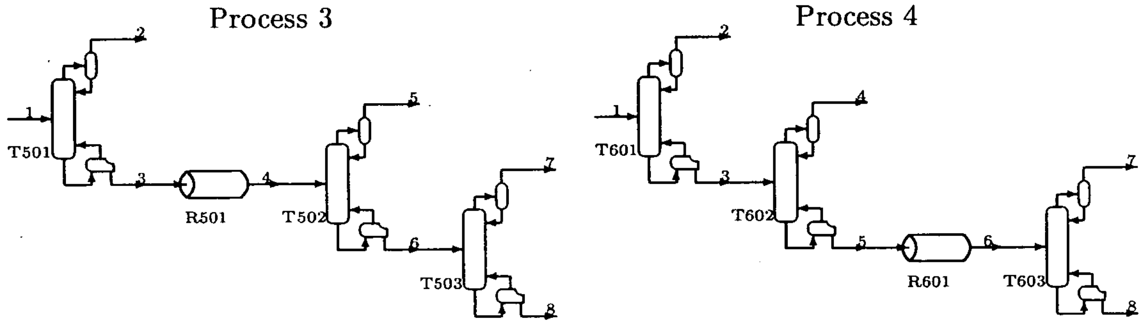
Process 1

Process 2



Process 3

Process 4

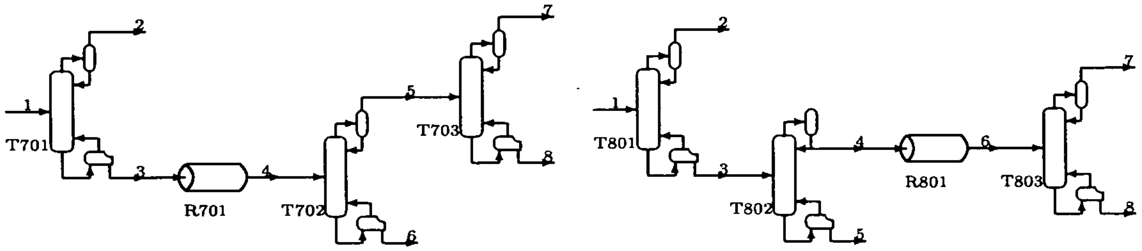


Process 5

Process 6

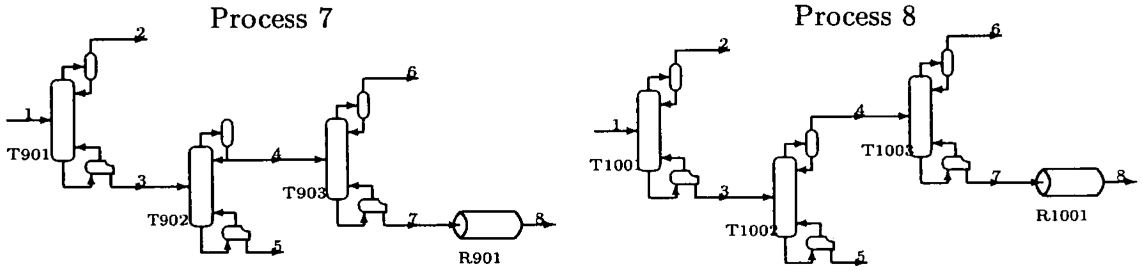
Figure 7.2: Synthesis Results

at the end of the system. This may prove to be hazardous to operate as the acetylene is distilled as a top product to a concentration greater than 98 mol % . We would expect that hazard to be highlighted in the study of safety. With liquid and vapour streams of acetylene present in processes 1 and 2 we will be able to identify any risks associated with chemical exposure. The main difference between process 1 and 2 is the selection of either a partial or total condenser. The main benefit of using a total condenser is that the system should be easier to control, however the synthesis stage has assumed that a total condensing column will be used when a lower specification is required. How to determine which systems can benefit from a low recovery will have to be analysed using the flexibility index as it is not obvious. If the system is being constrained by the separator then we would expect process 2 to have a lower flexibility



Process 7

Process 8



Process 9

Process 10

Figure 7.3: Synthesis Results

than process 1 with respect to disturbances in the feed concentration, therefore making the process easier to control.

Processes 5 and 7 have the hydrogenation reactor closest to the feed. This is likely to increase the cost of the reactor, but should bring about improved safety benefits as the acetylene is in its smallest concentration. These two systems also have the benefit that they will be able to produce the purest recycle stream.

It is interesting to note that the direct sequencing of separations used by process 1 and 2 is complemented by the indirect sequence of 9 and 10. The cost benefit of obtaining the correct column sequencing allows for 6 processes with the reactor placed at different locations within the separation sequence to be considered.

With each process producing very similar products it is difficult to see which is the most environmentally friendly. We would expect processes that manage to recover most of their product to be more favourable. Identifying the best process is difficult and something post synthesis should reveal.

7.3 Process Ranking

7.3.1 Costing

The costing returned in the synthesis stage is only a preliminary cost for the process. It would be useful to have an idea as to the cost associated with the process and the sensitivity of that cost to uncertainty in the design of the system and changes in the economic climate.

Because each process does return very similar product streams the variable forces in the cost analysis is the capital cost and the operating cost for each process.

7.3.2 Uncertainty in the Design Cost

Each design has a certain amount of uncertainty associated with it. In the ethylene study uncertainty lies with the energy requirements of each process and the capital costing. The revised costing enables us to examine the effect of a change in either the energy requirements or the capital cost for each process.

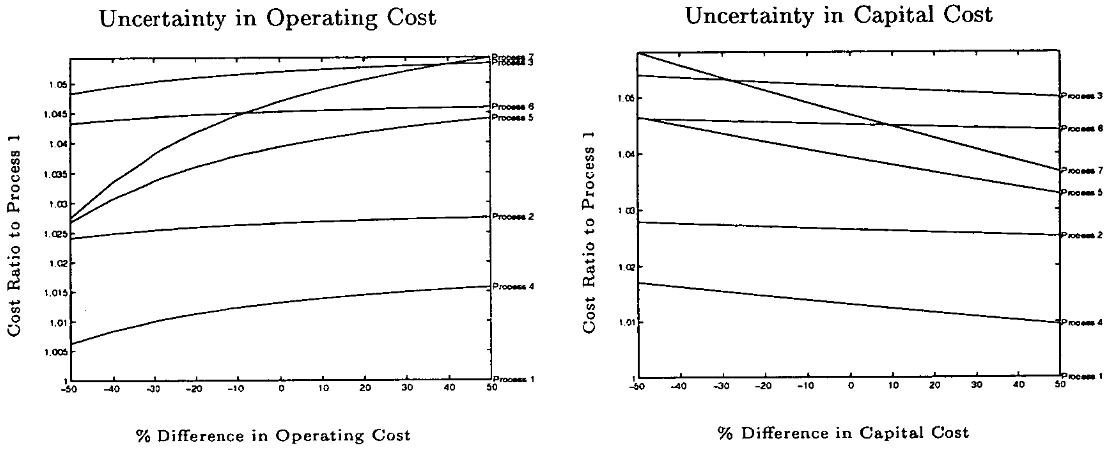


Figure 7.4: Uncertainty in Design Results

7.3.3 Changes in the Economic Climate

The Net present value is calculated at 0 % rate, so that the effect of the capital cost and operating cost can be seen. The results of this synthesis can be seen in figure 7.5. The cost is similar to the synthesis costing and the revised costing reorders the processes 1,4,2,5,6,3,7,8,9 and 10. Processes 8,9 and 10 have significantly higher costs associated with them than the other processes.

Process 1	2.970452e+06 $
Process 2	3.052440e+06 $
Process 3	3.129509e+06 $
Process 4	3.018364e+06 $
Process 5	3.103530e+06 $
Process 6	3.107197e+06 $
Process 7	3.135061e+06 $
Process 8	3.498001e+06 $
Process 9	3.512386e+06 $
Process 10	3.608943e+06 $

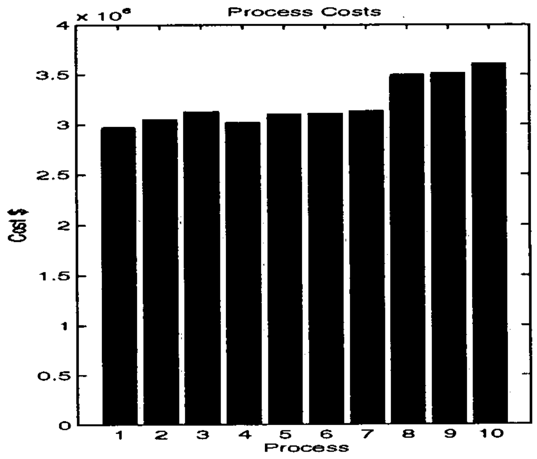


Figure 7.5: Process NPV at 0 %

Of greater interest is the effect of changing the interest rate that the NPV is calculated upon and the resulting change in cost. Increasing the interest rate increases the cost of each process, but some investments are more sensitive to this increase than others. Figure 7.6 shows the effect of increasing the rate. The graph on the left shows the effect upon each process, processes 1 to 7 have a similar value and differences are difficult to spot. The graph on the right highlights these differences by normalising the cost with respect to process 1 for these seven processes. From this we can see that process 7 is the most sensitive to changes in the interest rate, and at higher interest rates costs less than process 3 and 6. This is due to the fact that process 7 has the lowest capital cost, but this is offset by the cost of operation. Therefore the ability to delay cost can benefit the profitability of the plant.

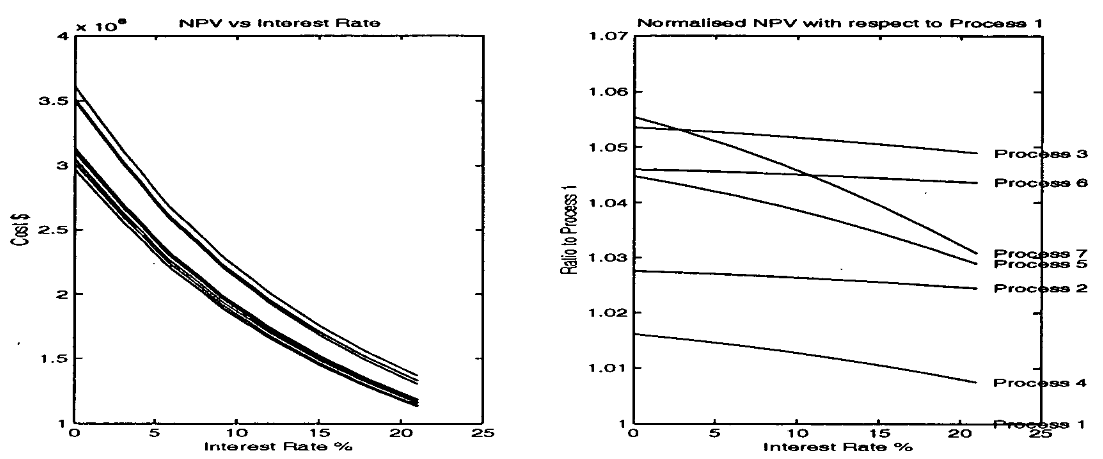


Figure 7.6: Process NPV at 0-21 %

7.3.4 Fire and Explosion Hazard Ranking

The operating conditions of each of the process alternatives reach extremes on both sides of temperature and pressure. Safety is a principle concern and choice of an inappropriate design will require extra provisions that can only be added at great expense. A review of each designs containment and operability control measures, methods of safe release of liquids and vapours, ignition prevention and incident prevention will enable the correct design to be chosen.

The fire and explosion index examines the last two criteria indicating how likely a major incident is to occur and if an incident does occur the likely damage that will result. Similar containment procedures and methods of release of liquids and vapours can be put in place for each of the designs. The scale of the ancillary safety equipment required is dependent upon the inventories being contained within each process.

The results from the fire and explosion index are returned in table 7.1. The index indicates that the hazards associated with each process are fairly consistent, and the process materials dominate the hazard associated with processing. The combined index indicated that processes 5,7 and 8 may have some desirable features, and process 7 is able to capitalise upon this lower index and produces the smallest damage cost at $ 38 million. Process 5 is similar in structure to process 7 apart from the fact that process

7 carries a lower inventory, therefore accounting for the $ 9 million difference.

Process	Process Total	C1	C2	C3	R1	Total Damage Cost ($)
1	170.3	43.3	41.7	42.6	42.8	57,500,000
2	170.3	43.3	41.7	42.6	42.8	57,200,000
3	170.2	43.3	41.7	42.4	42.8	57,600,000
4	173.0	43.9	43.1	41.1	44.9	46,500,000
5	166.5	43.3	41.2	40.9	41.1	46,000,000
6	170.2	43.3	41.7	42.4	42.8	58,100,000
7	166.3	43.3	41.0	41.0	41.1	37,700,000
8	167.2	43.3	41.7	41.2	41.1	45,600,000
9	172.6	43.3	41.7	42.1	45.6	60,700,000
10	172.6	43.3	41.7	42.1	45.6	62,600,000

Table 7.1: Fire and Explosion Indices

7.3.5 Chemical Exposure Ranking

The chemical exposure index functions as a screening tool and an index is returned for each stream in the process. An overall index is not returned for each process as that would encourage an entire system to be determined as safe or unsafe. Instead it is intended to highlight potential places within each design where hazards may exist providing that a sizable inventory is being held. The component exposure is given in appendix E.2.

Each component has an ERPG2 of 50000 showing that the main cause of concern is asphyxiation. Therefore, quantities and pressures of each component dominate the determination of the chemical exposure index.

The hazard distance for each feed stream is identical, however the operating pressure is variable hence the variations in the exposure index and the hazard distance between processes. Those processes which operate at a higher pressure have a larger hazard distance. For example processes 1,2,3 and 6 operate the first column at a lower pressure than the other processes and have respective lower hazard distances associated with them. The hazard distance has an upper limit of 1000 meters and streams that get to this upper limit should be examined in detail. The large hazard associated with the feed stream is due to the high pressure of the feed.

Stream	Exposure Index	Hazard Distance
1	188	1000
2	4.04	40.4
3	82.5	825
4	6.77	67.7
5	116	1000
6	5.96	59.6
7	77.7	777
8	59.3	593

Process 1

Stream	Exposure Index	Hazard Distance
1	188	1000
2	4.04	40.4
3	82.5	825
4	6.77	67.7
5	116	1000
6	117	1000
7	97.0	970
8	72.7	727

Process 2

Table 7.2: Ethylene Processes 1&2. CEI Results

Stream	Exposure Index	Hazard Distance
1	188	1000
2	4.04	40.4
3	82.5	825
4	6.77	67.7
5	116	1000
6	65.0	650
7	118	1000
8	98.6	986

Process 3

Stream	Exposure Index	Hazard Distance
1	188	1000
2	6.85	68.5
3	183	1000
4	6.45	64.5
5	85.0	850
6	65.9	659
7	7.17	71.7
8	144	1000

Process 4

Table 7.3: Ethylene Processes 3&4. CEI Results

If the designer wants to minimise the number of high risk streams and favour safe streams then we obtain 5 sets of processes which can be examined in detail. Processes 1 and 6 have the most desirable features with 2 streams requiring the maximum separation distance and 3 streams with a low separation distance. The two structures are similar with the placement of the hydrogenation reactor being the main difference. Because of the identical ERPG2 between components the conversion of acetylene has little benefit on the chemical exposure index and differences between the two systems is mainly due to pressure.

Processes 2,3,4,9 and 10 are slightly more hazardous with 1 more stream requiring the maximum separation distance. This increases hazard is mainly due to the increasing pressure of operation.

Processes 5 and 7 have 4 streams that are at the maximum separation distance. The

Stream	Exposure Index	Hazard Distance
1	188	1000
2	6.91	69.1
3	183	1000
4	116	1000
5	7.01	70.1
6	184	1000
7	6.75	67.5
8	96.3	963

Process 5

Stream	Exposure Index	Hazard Distance
1	188	1000
2	4.04	40.4
3	82.5	825
4	6.77	67.7
5	116	1000
6	65.0	650
7	6.86	68.6
8	94.4	944

Process 6

Table 7.4: Ethylene Processes 5&6. CEI Results

Stream	Exposure Index	Hazard Distance
1	188	1000
2	6.91	69.1
3	183	1000
4	116	1000
5	6.13	61.3
6	45.9	459
7	6.95	69.5
8	141	1000

Process 7

Stream	Exposure Index	Hazard Distance
1	188	1000
2	6.91	69.1
3	183	1000
4	183	1000
5	92.5	925
6	116	1000
7	7.02	70.2
8	184	1000

Process 8

Table 7.5: Ethylene Processes 7&8. CEI Results

pressure effect upon the chemical exposure index is most apparent when examining process 8 with each unit operating at the maximum operating pressure of 30 atmospheres, which will encourage pool formation of all the substances if a leak should occur.

7.3.6 Environmental Evaluation

Environmental evaluation can take a number of different forms and it is up to the design engineer to select the set that they consider to be the most important. Enhancement of the greenhouse effect, depletion of the ozone layer, human toxicity, ecotoxicity, photochemical oxidant formation, acidification, nutification and odour are the principle impact assessments to be carried out.

The chemicals involved in the production of ethylene have no significant impact upon

Stream	Exposure Index	Hazard Distance
1	188	1000
2	6.91	69.1
3	183	1000
4	82.6	826
5	41.9	419
6	6.77	67.7
7	113	1000
8	69.6	696

Process 9

Stream	Exposure Index	Hazard Distance
1	188	1000
2	6.91	69.1
3	182	1000
4	3.94	39.4
5	40.8	408
6	6.77	67.7
7	113	1000
8	69.6	696

Process 10

Table 7.6: Ethylene Processes 9&10. CEI Results

ozone depletion, toxicity, Ph imbalance or odour. So the designer will want to focus attention upon greenhouse emissions and photochemical oxidant formation. It is intended that the propane stream will be used as a fuel and all other streams will be either recycles or products then analysing the system with respect to photochemical oxidant formation will give us no useful information. The only index that may provide us with useful data is a study on the greenhouse effect. The greenhouse index can focus upon products or processes where the effect of the products are considered and their effect on the environment, or the process and the energy requirements of the system.

Looking first at the products from each system, the fuel stream is assumed to be completely oxidised and the components present are given a greenhouse rating compared to the amount of CO_2 that they produce. The more environmentally friendly plants will produce less CO_2 with respect to the quantity of products produced. The results of this greenhouse effect study is shown in table 7.7.

Process Number	Substitution/Elimination Index
1	0.105
2	0.105
3	0.104
4	0.122
5	0.103
6	0.104
7	0.0960
8	0.103
9	0.103
10	0.103

Table 7.7: Greenhouse Substitution/Elimination Index

The substitution/elimination index shows that there is very little environmental difference between plants. This is as we would expect as each process produces a similar product. In order to gain a true understanding of the greenhouse impact analysis of the amount of energy required in order to obtain this separation sequence needs to be performed.

Looking at the total amount of energy required by each separation column would give an indication as to the efficiency of the system, but this does not take into account heat integration and the efficiency of generating the utility required. The easiest way to account for this difference is to examine the cost of production of each utility. Higher value utility streams should require more energy to generate. Some of this cost must also be attributed into the capital cost of providing the utility. Cost is a suitable estimate to which processes consume the most energy, however only a life cycle assessment will provide all of the information.

Process 1	279069 $
Process 2	287297 $
Process 3	294802 $
Process 4	285057 $
Process 5	294282 $
Process 6	292330 $
Process 7	298742 $
Process 8	332917 $
Process 9	331053 $
Process 10	339932 $

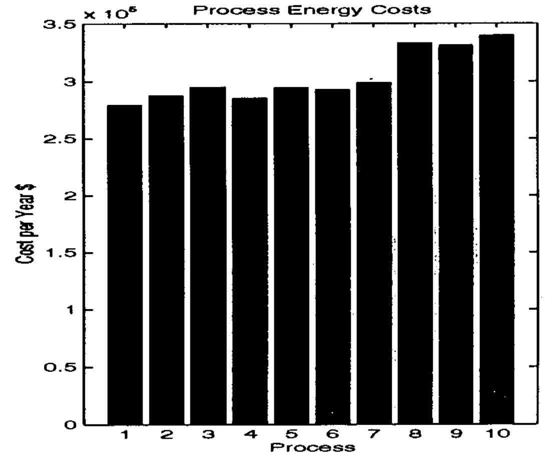


Figure 7.7: Process Energy Costs

From the cost basis there is more difference in the amount of energy required between the 10 processes. Because the operating cost of separation is the dominant force in the overall cost of each process the energy requirements follow the same pattern as the overall cost. There is a 22 % increase from the energy cost of process 1 to that of process 10.

The ranking for contributions to the greenhouse house effect is 1,4,2,6,5,3,7,9,8 and 10.

7.3.7 Flexibility

Processes 2,3 and 9 use one total condenser while other processes have a system of partial condensers. Therefore, it is desirable to know if this will effect the flexibility of the system and if so by how much. The Matlab flexibility files have been generated for each process with a variation in the feed concentration of 1 mol% for each component. The system is constrained by the original design constrains on product purity and physical constrains upon the system which are:

1. All component flows in streams must be greater than 0.
2. Principle ethylene product stream. Ethylene must be greater than 98 mol % .
3. Recycle stream. Ethane must be greater than 90 mol % .
4. Recycle stream. Propane must be less than 1 mol % .
5. Recycle stream. Flow must be greater than 10 kmol/hr.
6. Fuel stream. Propane must be greater than 80 mol % .
7. Low specification ethylene product. Ethylene must be greater than 88 mol % .
8. Low specification ethylene product. Flow must be less than 6 kmol/hr.

Table 7.8 shows the results of the flexibility index. As expected processes 2,3 and 9 all have a significantly lower flexibility index. All of the other processes have a very similar index and can reject disturbances to the feed on an equal basis.

7.3.8 Controllability

The design of the ethylene recovery system will have to cope with variations in the concentration of ethylene leaving the reactor. It is known that as the reactor is used

Process	Flexibility Index	Constraint Violated
1	2.0019	2
2	0.4260	7
3	0.9299	7
4	2.0018	2
5	2.0018	2
6	2.1817	2
7	2.0018	2
8	2.0019	2
9	0.5927	7
10	2.0019	2

Table 7.8: Flexibility Results with Variations on Feed Concentration

Process	Flexibility Index	Constraint Violated
1	0.3895	7
2	0.0730	7
3	0.1375	7
4	1.0006	1
5	0.8551	1
6	0.4289	7
7	0.8551	1
8	1.0006	1
9	0.0774	7
10	0.3867	7

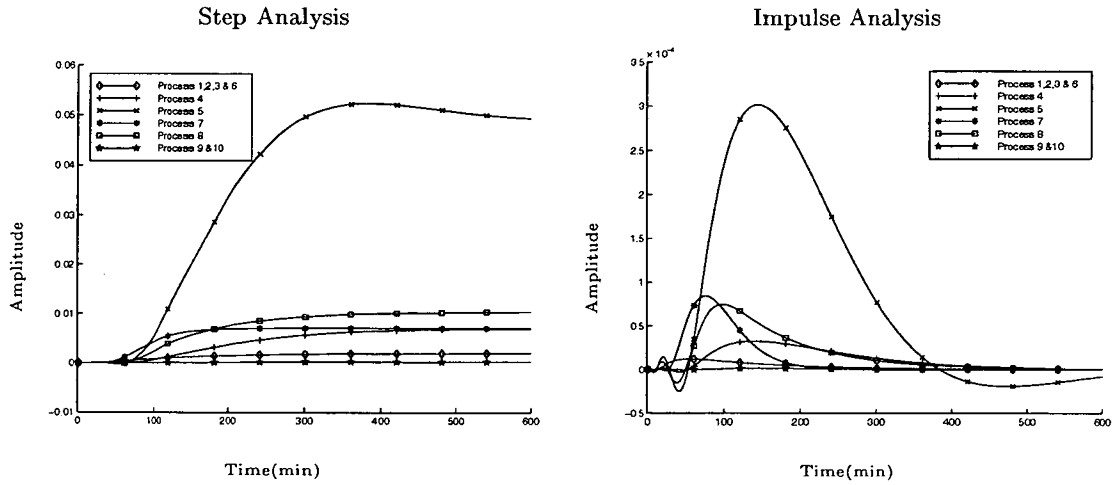
Table 7.9: Flexibility Results with Variations on Recovery

coke forms on the inside of the tubing hence reducing the conversion of ethane to ethylene, it is expected that sets of tubes will be de-coked using steam while fresh sets of tubes are brought on line. This will result in a step disturbance in the feed composition to the separation system.

Maintaining the correct product purity of the principle product is the main concern and it is useful to examine how differences in structure effect composition. Because the principle product is removed in the first column for each process with a very similar column it would be expected that the response of each process will be the same for the principle product and the focus can be upon other control issues.

The ethylene stream is used in a recycle and the concentration is critical in order to prevent cokeing of the reactor. Therefore, the first analysis of control will be to see how effectively the recovery system rejects disturbances. The control constants are shown in appendix E.5 which includes the time constants and the gains of each column with respect to ethane.

From these constants a transfer functions relating the output concentration to the feed concentration can be evaluated and the response of the recycle[1] to changes in the feed concentration evaluated. The response of the ethane recycle is shown in figure 7.8.


Step Analysis

Impulse Analysis

Figure 7.8: Ethane Recycle Analysis

---

[1] The recycle stream is stream 4 for Process 1,2,3 and 6, stream 6 for process 9 and 10, stream 7 for process 5 and stream 8 for process 8.

Processes 5,8,7 and 4 are the worst at rejecting disturbances, in particular the effect of 5 should be examined. Process 5 has the greatest inability to reject disturbances and will require the most careful control considerations with respect to the recycle to ensure that a cyclic build up of acetylene does not occur. Because the time delays for a disturbance to propagate through the system are long and the gain is small at 0.05, it is unlikely that the control issues would prove problematic and further analysis can be placed upon individual units.

7.4 Ethylene Study Discussion

The analysis of the ten processes has yielded some useful information about the design of an ethylene plant. The decision making process as to which of these designs is best is up to the designer. We can apply the four methods of decision making with multiple objective to highlight strengths and weaknesses of each design alternative.

7.4.1 Statistical Analysis

Analysis of some of the data that might be related could be useful in determining if the analysis can be reduced. Some of the measures for cost, safety, environment and control have been selected and are shown in table 7.10. This table forms an observation matrix to which the statistical analysis methods can be applied.

	NPV $*10^6$ \$ at 0 %	FEI Process Total	Total Damage $*10^6$ \$	Environment Sub/Elim	Environment Energy Cost $*10^6$ \$	Feed Flexibility	Recovery Flexibility
Process 1	2.97	170.3	57.5	0.105	0.279	2.00	0.390
Process 2	3.05	170.3	57.2	0.105	0.287	0.430	0.0730
Process 3	3.12	170.2	57.6	0.104	0.294	0.930	0.140
Process 4	3.01	173.0	46.5	0.122	0.285	2.00	1.00
Process 5	3.10	166.5	46.0	0.103	0.294	2.00	0.860
Process 6	3.11	170.2	58.1	0.104	0.292	2.20	0.430
Process 7	3.14	166.3	37.7	0.0960	0.299	2.00	0.860
Process 8	3.50	167.2	45.6	0.103	0.333	2.00	1.00
Process 9	3.50	172.6	60.7	0.103	0.331	0.590	0.0770
Process 10	3.60	172.6	62.6	0.103	0.340	2.00	0.390

Table 7.10: Case Study Result Summary

The observation matrix can then be transformed to give the covariance matrix so that the relationship between tests can then be examined.

The eigenvalues and correlation matrix of the covariance matrix can then be evaluated and is shown in equation 7.1. From this it can be seen that two of the eigenvalues are zero and therefore there must exist a linear relationship between three of the the observation tests.

$$\underset{\text{Eigenvalues}}{\begin{pmatrix} 0.0000 \\ 0.0000 \\ 0.0004 \\ 0.0065 \\ 0.0119 \\ 0.0688 \\ 0.6482 \end{pmatrix}} \quad \underset{\text{Correlation Matrix}}{\begin{pmatrix} 0.7087 & 0.1521 & 0.2009 & -0.0934 & 0.6522 & -0.0091 & -0.0066 \\ 0.1017 & -0.9297 & 0.3282 & 0.1297 & 0.0235 & -0.0111 & -0.0087 \\ -0.0077 & -0.1164 & -0.6166 & 0.6421 & 0.3120 & -0.2696 & -0.1543 \\ -0.0320 & 0.3084 & 0.6098 & 0.7183 & -0.1215 & 0.0345 & 0.0154 \\ -0.6973 & 0.0053 & 0.2283 & -0.1139 & 0.6698 & 0.0009 & -0.0026 \\ -0.0055 & 0.0354 & 0.1293 & -0.1032 & -0.0647 & -0.8813 & 0.4364 \\ 0.0061 & -0.0510 & -0.1763 & 0.1504 & 0.0954 & 0.3862 & 0.8862 \end{pmatrix}} \tag{7.1}$$

By examining the correlation matrix a relationship can be seen between cost and the environmental energy cost. This could be expected as operating costs contribute a significant part to the profitability of the process. An increase in cost is associated with an increase in the energy costs means that further analysis of the energy cost is not necessary.

Reexamination of the test results shows that the variance of the substitution/elimination analysis is small. Most of the points lie about the .104 range and there are insufficient points in this analysis to proceed with this data set. Therefore, the substitution/elimination index can be eliminated from this analysis.

The eigenvalues can then be reevaluated with the reduced observation matrix and the results are shown in equation 7.2.

$$\underset{\text{Eigenvalues}}{\begin{pmatrix} 0.0001 \\ 0.0027 \\ 0.0069 \\ 0.0688 \\ 0.6480 \end{pmatrix}} \tag{7.2}$$

From this it can be seen that flexibility has the greatest variation on the analysis and that cost only has a small variance.

7.4.2 Dominance

The rank for each of the indexing methods that has been used is shown in table 7.11. The table shows that the processes are distributed in their rankings and there is not one processes that can be selected as being dominant over all of the other processes. Therefore, there is a case for applying the tools of multiple-objective optimisation to find the most suitable process.

Synthesis Cost	Cost with a -10 % Operating Cost	Cost with a +10 % Operating Cost	NPV at 10 %	Fire and Explosion Index	Chemical Exposure Index	Greenhouse Index	Feed Concentration Flexibility	Recovery Flexibility	Recycle Control
1	1	1	1	7	1	1	6	4	9
2	4	4	4	8	6	4	1	8	10
3	2	2	2	5	2	2	8	5	1
4	5	5	5	4	3	6	10	7	2
5	7	6	7	2	4	5	4	1	3
6	6	7	6	1	9	3	5	10	6
7	3	3	3	3	10	7	7	6	4
8	8	8	8	6	5	9	3	3	8
9	9	9	9	9	7	8	9	9	7
10	10	10	10	10	8	10	2	2	5

Table 7.11: Case Study Rankings

7.4.3 The Efficient Frontier

The question as to whether or not any process can be eliminated because it fails to make an improvement in at least 1 criteria. This is the simplest method of multiple criteria decision making and requires examination of the ranking of each indexing method as given in table 7.11.

From the table of case study ranking processes 1,7,6,4 and 9 have the best rankings for at least one of the indices. All of the processes from 1 to 8 have to be included in the analysis as they make an improvement in cost compared to process 9, therefore leaving process 10 as the only process that could be eliminated due to dominance. However, there is a significant improvement in the feed concentration flexibility of process 10 compared to process 9 and therefore it would be inappropriate to eliminate this process.

The Efficient Frontier can be a useful tool for eliminating processes from the design set, however as the number of indexing methods is increased the ability to eliminate a processes becomes more unlikely. In this case no processes can be eliminated and the study would have to proceed with the assumption that each of the processes was valid or a value based assessment of the alternative would have to be made.

7.4.4 Lexicographical Ordering

To apply lexicographical ordering requires the assumption that there is a degree of uncertainty associated with each of the rankings and a degree of tolerance between designs, it is only possible to examine trends in the design. A tightly constrained system focuses upon the preliminary cost of the systems and results in the processes lying in the original order. By slackening the tolerance more processes become equally valid and further criteria have to be used to differentiate between processes. The order of importance for each process is critical and in the ethylene case one criteria rank is to have cost being of prime importance followed by fire and explosion safety, chemical exposure, environmental issues and finally flexibility.

Considering a 10 % uncertainty in cost results in processes 1 to 7 being equally valid and a second inferior set of processes 8 to 10 also being equally valid. We therefore have two sets of processes that we will want to examine in more detail. The second most important criteria after cost that should be examined is the influence of each process upon safety. A 10 % uncertainty in the fire and explosion index fails to separate up the processes any further. The total damage that can be caused by each plant does separate the plants to a greater extent. Process 7 has the lowest potential damage of \$ 37,700 and a 10 % uncertainty in this figure means that any process that causes less than \$ 41,470 worth of damage would be equally rated. There are no processes that meet this criteria and process 7 is therefore ranked as the top process. The analysis could stop here and accept that process 7 is the ideal process, or the ordering can be expanded to include the rest of the processes until a list of rankings is achieved.

Selecting from process 1 to 6 the next process with the smallest total damage is chosen. Process 5 has a total damage of \$ 46,000 and all processes with a damage of less than \$ 50,600 are therefore equally valid. Therefore process 4 is equally valid. This process continues with all of the remaining processes 1 to 7 and then applied to the set of inferior processes 8 to 10 and the following rank is obtained.

$$7 > 4,5 > 1,2,3,6 > 8 > 9,10$$

The next most important criteria is to minimise the potential exposure to high risk streams. The ranking of the processes with respect to chemical exposure is process (1,6),(2,3,4,9,10),(5,7),8. The lexicographical ordering of the processes is then split further up so that process 4 ranks higher than 5, and processes 1 and 6 rank better than 2 and 3.

Examination into a 10 % difference in the environmental issues fails to separate the processes any further. A 10 % analysis into the flexibility of each system with respect to the feed concentration separates processes 3 and 2 with 3 being the more favourable process, and also separates process 10 and 9. The variation on recovery fails to differentiate between processes 1 and 6 and therefore under this analysis and with these tools that are available the analysis is unable to differentiate any benefit between process 1 and 6. The final ranking of the processes is.

$$7 > 4 > 5 > 1,6 > 3 > 2 > 8 > 10 > 9$$

This system of analysis is very dependent upon the values of each index, and the degree of tolerance associated with each result.

7.4.5 Indifference Curves

There exist two methods for the ranking of processes.

1. Weighted Position Ranking (WPR).
2. Ranked Value Judgement (RVJ).

The easier of these is Weighted Position Ranking where a value is placed upon the position in the ranking chart that each process attains. A simple method is to sum the position of each processes for each rank with the best process having the lowest total giving the following ranking 1,4,2,6,5,7,3,8,9,10. The main disadvantage with this is that it does not reflect the actual value associated with each rank. This can be very misleading as it is weighted in favour of the less important methods. A better method is to value each rank and multiple the inverse of the value by the position of each process.

	Value
Synthesis Cost	0.5
Cost with a -10 % Operating Cost	0.5
Cost with a +10 % Operating Cost	0.5
NPV at 10 %	4
Fire and Explosion Index	3
Chemical Exposure Index	2
Greenhouse Index	1.5
Feed Concentration Flexibility	1
Recovery Flexibility	0.25
Recycle Control	0.5

Process	Process Value	WPR
1	37.4	1
2	79.9	4
3	94.1	8
4	44.7	2
5	73.3	3
6	82.8	5
7	87.8	6
8	88.7	7
9	114.6	10
10	108	9

Table 7.12: WPR Analysis

7.4.6 Ranked Value Judgement

Ranked Value Judgement is the most complicated method of all the post-synthesis methods. It considers alternative ranking methods simultaneously and utilises the values associated with each of the ranking methods. However, the method is dependent upon understanding the trade offs between different criteria.

RVJ is easy to visualise in two dimensions and figure 7.9 has the two criteria of cost and safety plotted for each process. Also shown on the graph are lines of equal utility which are made up from knowledge of the trade off between the total damage cost and the synthesis cost. In this case the trade off value is set at 1 to 1000, i.e. a $ 1 increase in cost to save $ 1000 worth of damage. Process 1 lies on the line of maximum utility and is therefore the most desirable process.

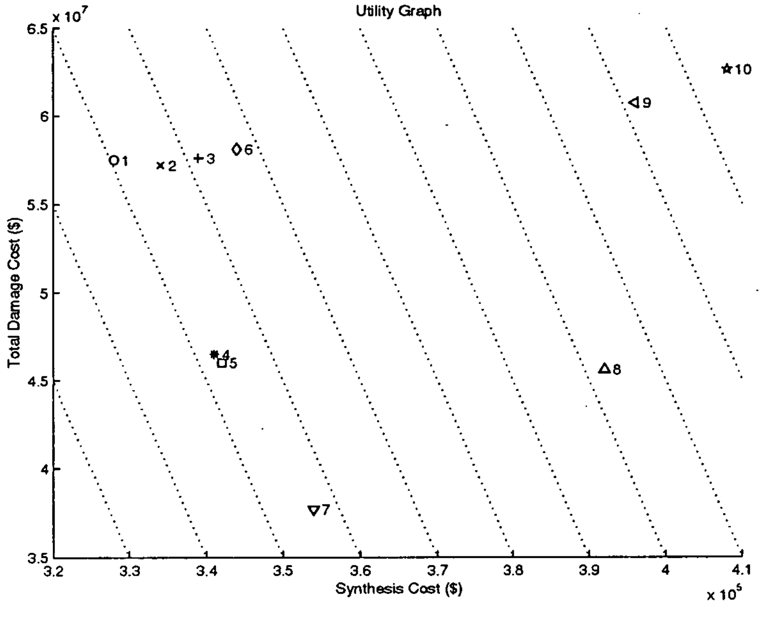


Figure 7.9: Safety/Cost Utility

With RVJ and using these two criteria we can see that process 1 4 5 and 7 are all valid depending upon the trade off value chosen. As the safety criteria is increased in importance processes 4 and then 5 become desirable processes until the value of safety is doubled to 1 to 500 then process 7 becomes the most desirable.

This method does highlight the fact that processes 8 9 and 10 are so far behind the other 7 processes in their utility value that they would have to excel in other ranking methods before they would be taken forward for further design.

Applying this method to more than 2 criteria becomes difficult as the trade off between each ranking methods needs to be established. Methods like the chemical exposure index do not provide quantifiable ranked values that can be used by this method and therefore has limited use.

7.4.7 Design Development

The post synthesis methods have indicated where problems may occur in the design and the post synthesis optimisation tools have helped to confirm these indications so that the design can focus upon those processes of interest. The optimisation tools show that the designer should be looking at processes 1,4,5,6 and 7. At the beginning of the design it was expected that problems would occur with the acetylene concentration and processes 1 and 6 would be eliminated. While the system has not eliminated these two processes it has highlighted the differences between these processes and shown the potential advantages that they have including cost and chemical exposure advantages.

Chapter 8

Discussion and Conclusions

8.1 Discussion

Foresight in the design process can help to increase the efficiency of development of a design. Few designs out of many considered become a reality and being able to select the best process early on in the design procedure can reduce the time spent developing inferior solutions. Process designs can fail to be implemented for a number of reasons and selecting the best process requires a broad understanding of the characteristics of each process alternative. Also each design is different and has particular design problems associated with it. The procedure must therefore be flexible and extensible, and to save time this analysis is best performed early on in the design process. This thesis has developed an analysis procedure which includes applications that can help predict the properties of a conceptual design and highlights their suitability.

The analysis procedure works with the generated flowsheets from the synthesis stage of the design process. Figure 8.1 shows the scope of the post synthesis analysis procedure, which assesses feasible process designs and continues to the point where the development of detailed designs can be made. The post synthesis tools available to the designer can either analyse each process to help the user determine the characteristics of each process (Analysis Tools), or they can evaluate each process to provide a process ranking (Evaluation Tools). The procedure uses the results from the post

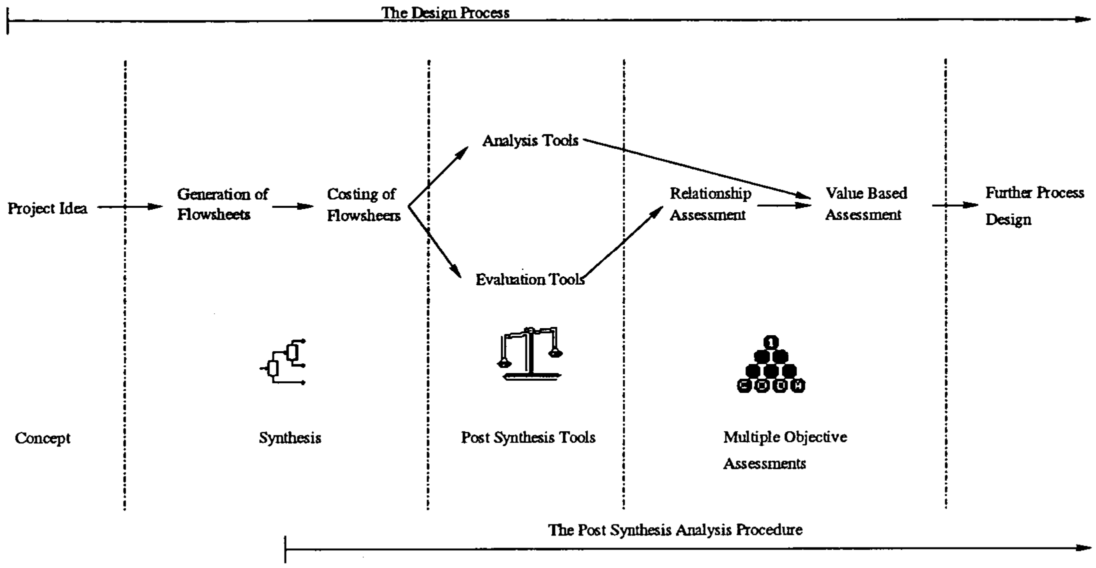


Figure 8.1: The Design Process

synthesis tools and ranks them using multiple objective assessments. Evaluation tools that provide a quantifiable result about the suitability of a process can be assessed using relationship assessments, such as statistical analysis. If the characteristics of the process have been determined using an analysis tool or the relationship assessments fail to show the most desirable process alternative then value based assessments have to be used. This procedure should highlight the suitability of a process and enable the designer to perform a wider search of process alternatives.

Difficulties occur in developing tools that are efficient, produce meaningful results and are applicable to conceptual design. The procedure developed in this thesis has addressed these problems by using a management system for the process data combined with the user's own input. Analysis tools have been developed that can quantify decision making and record the rational behind the decisions. With this information available future designs can examine the design process of previous plants and when new technology emerges the knock on effects seen, and entrenchment of old design practices avoided.

The first stage in design is to generate a set of process alternatives. These could either be generated by the user or created using a synthesis package. The synthesis method employed in the hydrogen cyanide case study in chapter 6 and the ethylene case study in chapter 7 is a branch and bound method using the CHiPS [23] package. Alternatively processes could be created and entered into the system by the user, using either the Douglas [3] hierarchical approach or utilising data from existing processes. Once the process structures are known, multi-objective synthesis where criteria different to cost can then be considered. This could be carried out at the same time that the processes are generated, but as has been discussed in section 2.2, this can only be done quantitively if the value function between conflicting objectives can be explicitly defined. Instead, the method we have developed generates alternatives based upon one criterion and then subsequently evaluates according to other criteria. The CHiPS package generates different process alternatives and ranks them according to cost. Cost could be substituted for other ranking criterion providing that it is quantifiable and accumulative.

8.1.1 The Procedure Environment

The post-synthesis procedure requires a management system which has been discussed in chapter 3 which governs not only the look and feel of the system developed, but also its extensibility. The management environment that has been used, has been developed by Andrews [21] using the World Wide Web to contain unit data and link into external databases. This provides the flexibility required and enables a wide range of development tools to be added to the system to suit the needs of individual designers.

By having an effective management system applications can be applied to either one or a collection of processes. The system has been created so that applications which analyse the heat and mass inventory for individual processes are generated by the `topology` object, while further indexing methods analyse groups of `topology` objects connected together through a class object. The advantage of this is that groups of processes can be analysed together and the results recorded for future use.

For each process the management system has a topology object holding together `streams` and `units`. During the development of post synthesis tools it has been found

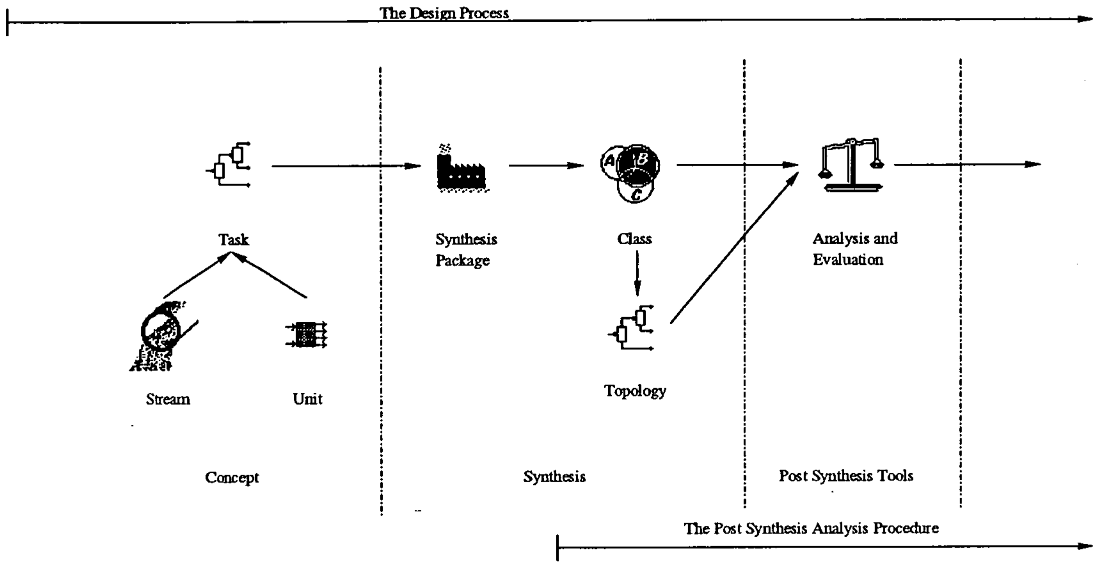


Figure 8.2: The Design Process Environment

necessary to expand the number of objects in the system so as to cover the range of data required for post synthesis analysis. For example, a `task` object has been included which connects `streams` and `units` together and formulates the input to the CHiPS synthesis package.

Conceptual designs contain the outline of the process, with much of the desirable information not known, such as ancillary equipment, materials of construction and control structures. In many situations this information governs the feasibility of a process design. The management system solves this problem by enabling databases to be linked to the package so that assumptions can be made about the potential possible final design. For example the flammability of components has not been used at the synthesis stage of design but the components present are known. The system contains links back to a database of `statistic` objects where the information about the flammability of each component is contained. While it might seem that this complicates the structure of the system, it enables multiple processes to be analysed with only one `statistic` object being created and maintained. By containing extra data as a separate `statistic` objects within each `stream`, `unit` and `component` more efficient data mining is possible. For example, analysis methods that require extra component data but not extra unit data can extract the `component statistic` object only.

Being able to identify how a result was generated is important as different processes are analysed. If a self contained application had been created then the input file and the generated result would have to be tied together. While it might be obvious that the file *result1.txt* was the output from *input1.txt* confusion can arise when multiple files are being analysed. The web based system removes this ambiguity through the use of hyperlinks to other web objects where the history files are recorded along with information as to how the objects are related. Being able to find the original source of the data is advantageous, but because it can be cumbersome `report` objects are generated every time a post synthesis analysis is carried out. `Reports` records the location of the `statistic` object and the data value used in the calculation. This enables the designer to examine all of the data being requested from the database which is important when multiple users have access to the system and consistency in the analysis needs to be maintained.

8.1.2 The Post Synthesis Tools

Post synthesis analysis tools incorporated into the system have been described in chapter 4. There are two types of analysis methods, tools that reassess the processes on an index basis and provide a quantifiable result (Evaluation Tools) or tools which connect to external packages and allow the user to explore the characteristics of a process (Analysis Tools). Some tools are a combination of analysis and evaluation depending upon how the user implements them. The post synthesis tools that have been developed are:

- Cost (Analysis/Evaluation)
- Safety (Evaluation)
- Environment (Evaluation)
- Flexibility (Analysis/Evaluation)
- Dynamic Control (Analysis)

Costing Analysis

Cost is the primary indicator of the suitability of a process design, but the analysis has shown that synthesis costing will be replaced during the course of design starting with simple direct costing going through to obtaining the true cost figures from suppliers. Obtaining accurate cost estimations is important so that the benefits of different alternatives can be made. While true cost figures from previous designs would be the most desirable alternative, this information is not always present, especially in the case of development of a new design. This thesis shows that costing methods that are used must be chosen carefully as different costing measures produce different results. The simplicity and transparency of direct costing makes it ideal for synthesis, but this can be improved as conceptual designs contain enough information to apply a discounted costing analysis. Section 4.1.5 shows that applying discounted costing can change the apparent profitability of the process.

The costing tool demonstrates many of the features and benefits of the post-synthesis analysis. Costing can be considered as an evaluation tool as it returns a number of results including:

- Direct Cost
- Pay-back Time
- Net Present Value
- Internal Rate of Return

Each of these indexing methods will give a different value and can alter the process ranking. Therefore the costing analysis can also be used as an assessment tool. The procedure has been developed to be informative and allows the user to examine the process costing using a spreadsheet. The capital cost, operating cost and the process inventory can all be collected together in the spreadsheet and cost analysis can be made of:

- Capital Cost Sensitivity
- Operating Cost Sensitivity
- Uncertainty in Market Conditions
- Uncertainty in Process Conditions

The cost indexing procedure also demonstrates the need for the post synthesis applications to interface to the synthesis input. The web environment allows the original synthesis task file to be hyper-linked to the process results and hence is available to the post-synthesis tools. This means that costing information used at the synthesis stage can be extracted and incorporated into post-synthesis analysis ensuring consistency in the design procedure. The spreadsheet format also enables the design to progresses with further cost revisions made in a spreadsheet similar to the one used for the conceptual analysis.

The cost uncertainty of a process can be examined and section 4.1.5 shows the cost effect of changing conditions upon two processes. Changes to the interest rate along with differences in operating cost and capital cost have been examined. The initial cost estimates are made at an interest rate of 0 % . From the analysis it can be seen that as the interest rate is increased then the profitability of both processes decrease and if the interest rate is high enough the process ranking becomes reversed. However, no process operates in a stable environment and this can be examined as the spreadsheet incorporates a linear model of the process. Changes to the process inventory can be made along with changes of capital cost and the operating costs, at varying interest rates to give the profit sensitivity of the process. The cost analysis has shown that:

- Selecting the correct cost measure is important so as to understand the profitability of each process.
- Post synthesis tools require an interface to the synthesis information.
- By using a spreadsheet format, evaluation tools can also be used as analysis tools.

Safety Analysis

The design of an inherently safe process has to be examined at every stage of the design procedure. At the conceptual level this is addressed by trying to eliminate process hazards from the system. Ideally a Hazop study would be employed, but with much of the design unknown this could provide a false sense of security as potential hazards are ignored. Instead concept hazard analysis needs to be used to address specific hazards and examine if he system could be designed better. The two evaluation tools that have been proposed in this thesis are the Dow fire and explosion index in section 4.2.4 and the chemical exposure index in section 4.2.5.

The Dow fire and explosion index [39] is probably the best well known of the indexing methods. Assessment of the flammability and explosive potential of streams is calculated along with the damage cost if a flammable loss was to occur. Because the format of calculating the index is well defined for a detailed design, assumptions have had to be made and a simplified version used for conceptual level design. For example the effect of corrosion is assumed to be constant for each process analysed. The system enables reviews of these assumptions to be made by maintaining the same format of analysis as detailed design.

Conceptual design is well suited to examining inherent design features as the processes do not have any safety equipment present. The index is calculated on a unit basis, but requires the potential hazard of each stream connecting to the unit to be identified by the components material factor. Once the potential hazard is known the risk of loss can be calculated to give a final fire and explosion index. This gives an overall evaluation for the whole process along with an index for each unit and a total damage cost for the entire process.

The fire and explosion index applied to the ethylene case study in section 7.3.4 shows how the procedure can be applied to a number of processes. The benefits within each process can easily be seen, and either be exploited or the design modified to remove the hazard. The ethylene study in section 7.3.4 shows that differences between the total damage cost and the total process fire and explosion index can lead to different process rankings. The cost and inventories held within each process unit are used to evaluate the total damage cost, therefore resulting that processes with a high index but a small inventory can be considered safer than some units that have a large inventory and lower index associated with them.

The release of toxic materials has also been considered with an index similar to the fire and explosion index. The Dow chemical exposure index [41] shown in section 4.2.5 assesses the potential release impact from toxic materials contained within each process, by assessing the potential rupture of pipes in the process. To perform this calculation the analysis tool requires the pipe size of every pipe in the process, the contents of the stream and their human toxicity. The pipe size is collected from the `stream statistic` object, but if it is not known a separate post synthesis application can be applied to size the pipe work described in section 4.4. This shows that the procedure can connect together the result from one analysis tool to the input of another analysis.

The exposure index must determine the amount of material that could potentially be released into the atmosphere. Because the properties of a stream change upon release, the analysis has to have access to a thermo-physical property package so as to determine the phase of the release and the amount released. The modular approach of the management system connecting tools and databases together enables the same physical property package which has been used for synthesis to be used by post synthesis analysis tools.

Once the airborne quantity released is known the hazard distance can be calculated. The index returns a hazard distance for each stream which is useful in determining the safety distance required. To obtain an index for each unit a pessimistic view has to be taken by considering the stream with the greatest index connecting to the process unit. This has been examined with a study into the benefits of separating one heat exchanger into a two heat exchanger system which can be seen in section 4.2.6. The analysis shows that by reducing the area of the pipes the overall required safety distance can be reduced, but the cost is increased. Applying the safety study requires that:

- Conceptual safety analysis has to be aimed at a specific hazard.
- The analysis tool must have access to a safety database.
- Assumptions that are made in the evaluation need to be reassessed.
- Connections to other assessment packages is essential.

Environment Analysis

Environmental indices are very specific to the process being designed and a number of alternative environment indexing tools have been proposed. The evaluation tool developed allows quantifiable environmental measures to be made of some issues. Measures are based around the life cycle assessment of the process, which is an auditing assessment performed around the inventories of heat and mass entering and leaving the process. The procedure is well suited to this analysis as the input-output information is well defined for a conceptual design and the data is easy to extract. It has also been shown that if the process can only be improved by eliminating a waste or turning a waste into a useful product then the substitution/elimination index can be used to help quantify the environmental impact. This can be useful when considering similar processes of varying scale. The environmental study in section 4.3.5 shows the benefits of using both indexing methods. The environmental study shows the potential for process improvements which can be seen in the substitution/elimination index and the cause of the environmental impact which can be identified using the life cycle assessment.

Quantifiable environmental measures have been discussed in section 4.3 and include enhancement of the greenhouse effect and depletion of the ozone layer. The analysis requires information about the quantity of components present, their effect upon the environment and the method of release. Because the final destination of streams leaving the system is likely to affect the environmental index the `stream statistics` are examined to find out the stream destination. For example, streams that leave the system as a product or are to be incinerated can have a different index than those that enter the environment directly through a sewage stream or purge. The key points of the environmental tool is that:

- Different analysis methods can give different environmental impact results.
- The final destination of process streams can affect the environmental impact.

The global warming potential of the hydrogen cyanide case study in section 6.2.4 demonstrates the need to use the environmental study with care. The substitution/elimination index would indicate that one process is much better than the other two alternatives. However upon closer inspection of the life cycle assessment the processes are significantly different with respect to the quality of the final product. If the quality of the product can be improved then the environmental impact can be reduced.

Flexibility and Control Analysis

The most complicated assessment tools are those that assess the controllability of the chemical process. The method proposed considers these under two headings:

Steady state control analysis examines the limitations of the design parameters and how the system rejects disturbances

Dynamic control analysis enables predictions about the behaviour of units from their operating parameters to be made.

Steady state control analysis is the simplest of the control analysis methods. By examining the boundaries of operation where the system becomes infeasible the flexibility of the process can be established. The method involves using a model of the system and disturbing control issues until the system becomes infeasible. this assumes that the process operating bounds lie in a convex space and the bounds lie at the extremities of the control issues. The flexibility index is governed by the users choice and magnitude of disturbance as shown in the flexibility development study 4.5.3.

The flexibility study has demonstrated the need for the system to interface to a mathematical analysis package. An input file for the Matlab package is generated, but any mathematical package or spreadsheet could of been used. The Matlab package is especially useful because of the efficient handling of sparse matrices and graphing tools available. The analysis works around a linear model of the process resulting that disturbances have to be kept small to ensure the model remains feasible. It has been shown that if the model is made more complex convexity of the feasible operating region cannot be guaranteed. The only way to find the true flexibility of the process is to perform a rigorous search around the boundaries of feasibility. Because this requires a high level of computation to gain just a little information, it has been proposed that the flexibility is assessed by examining a linearised approximation of the system. This can then be re-evaluated at the limit of feasibility to test to see if the system is still valid.

Dynamic control assessments can made either by using a linearised approximation of the system or by examining the resilience of a dynamic simulation with the units control structure in place. While dynamic simulation is the most informative method and covers a wide range of situations including startup and shutdown, it requires detailed knowledge of the system. At the conceptual level the required information is not present as it includes information about the control structure.

Because much of the control structure is not known linearised approximations can be made about the response of the system described in section 4.6.3. This has been done by using a transfer function for the system which relates the expected disturbance to the effect upon the output. Modelling the response in the Laplace domain enables transfer functions to be linked together much like a topology. This means that complicated systems can be modelled using a collection of transfer functions. This has required the creation of two more objects in the management system of a `control` object and a `transfer function`.

Measuring the controllability of a process has required defining the control objectives. These have been defined to be that certain measures should be kept at a desired level and that a measured value should follow a time varying reference. It has been proposed that these can be measured by the minimum squared error between set point and output and the time taken for the system to reach steady state. Analysis of control between the dynamic simulation and the linearised approximation has been considered and the results show that differences do occur. While the general trend is similar between results, the magnitude of the output and the time taken to reach steady state can vary enormously. It would be desirable to obtain similar results the linearised approximation assessment can prove to be useful when used as a screening tool for control.

Analysis Tools Summary

The tools developed demonstrate the ability of the assessment tools to interface with external packages and the need for the procedure to connect to external databases. The cost analysis demonstrates the need to connect to the synthesis input data and produce a spreadsheet package. The safety analysis shows the need that post synthesis analysis needs to be consistent with future designs so that errors in the design can be traced back to the conceptual level. Safety analysis also requires access to an external database about the hazard of components present and an interface to a physical property package so that further analysis can be performed. The environmental analysis shows that even when a simple auditing tool is required the input of the designer is still required. Control demonstrates the need that the package has to be flexible so that transfer functions can be produced and the need to connect to a mathematical package such as Matlab. These packages demonstrate the flexibility and extensibility of the system. The applicability of these methods has been tested in the hydrogen cyanide case study and the ethylene case study.

8.1.3 The Case Studies

Hydrogen Cyanide Study

The hydrogen cyanide study in chapter 6 examines three processes, and is particularly interesting because of the recycle loop of ammonia and methane, which adds to the complexity of the problem. Each of the process systems has a large utility requirement that dominates the final cost. The main issues other than cost associated with the design of a hydrogen cyanide plant are safety, environment and controllability issues.

The fire and explosion index shows only a small difference between process alternatives, but once the index is calculated, the units affected and the maximum probable damage caused can be seen and differences between the processes can be examined. The study shows that care needs to be taken when examining the index, but certain conclusions can be gained. The analysis has shown that any unit which processes hydrogen cyanide has an increased risk of fire and explosion, and the dilution of hydrogen cyanide streams with ammonia can reduce the fire and explosion hazard.

Applying the chemical exposure index to the hydrogen cyanide processes reveals large differences in the safety of the product stream. The analysis can highlight certain areas and demonstrates that the safety of the system is governed by the streams leaving the distillation system. The analysis also shows that high pressure vapour streams should be avoided which occurs in the second hydrogen cyanide process.

The environmental study has examined the global warming potential of each process. The environmental study has shown that life cycle assessment is the most appropriate environmental measure when considering similar processes which results in process 3 and 1 being favoured over process 2. The study has shown that the substitution/elimination index has to used with care as it been distorted by a large index in the product stream of process 2.

The flexibility of the hydrogen cyanide systems is examined by disturbing the feed composition, the recovery and the extent of reaction. Depending upon the chosen disturbed variables and the values of the expected disturbance results in differing values for the flexibility index. Repeated analysis of the flexibility index has shown that the second process is constrained with respect to recovery in the distillation column and therefore more care would have to be taken when designing the distillation control structure.

With three process being analysed it has been possible to compare the linearised approximation of the reactor, distillation and flash model to dynamic simulations. From this it can be seen that the linearised approximations show the correct gain and trend of response that would be expected, but differences do occur between the two methods. This shows that the linearised approximation gives indication as to the possible control problems but cannot substitute for a full dynamic simulation.

The hydrogen cyanide study has shown that different indexing methods favour different processes and the designer has to be specific in the characteristics that they wish to examine. The procedure has enabled the amount of conflict between criteria to be assessed and enables a design decision to be made based upon the users own personal preference.

Ethylene Study

The ethylene case study in chapter 7 shows the benefits of applying post synthesis procedure to a large set of processes. The study has considered the separation section of an ethylene process to produce two ethylene products, a recycle stream and a heavy oil stream. Most of the design differences focus around the location of the acetylene reactor.

The cost analysis has shown the benefits of a spreadsheet in which the user can adjust, for re-evaluating the cost analysis. It has also been demonstrated that the process ordering can be affected by introducing more accurate costings. The cost analysis has been used to examine uncertainty in the operating and capital cost of the process at varying interest rates. The ethylene study shows that certain processes are very sensitive to changes in the interest rate, and that reduction in the operating costs can have the potential to dramatically influence the profitability of some of the processes.

The fire and explosion analysis shows that the process materials that are present dominate the safety factor. Some processes are able to capitalise upon this by having a high index at a point where there is a low inventory of flammable materials present. The index does change the order of the processes and shows that inherent safety does come at a price.

The environmental evaluation of the different process alternatives requires post synthesis analysis as all of the streams produce similar products. The environmental analysis has examined the global warming potential of each process and proves that all the processes have a similar influence upon global warming with respect to their products. Relationship analysis also shows a positive linear relationship exits between the environment index and cost, therefore only cost indices need to be considered further.

The flexibility index has analysed the effect of varying the feed concentration and the recovery in the distillation columns. The analysis has shown that some processes are capable of rejecting the expected disturbances while other processes are constrained by the product constraints or limits on the linear approximation. The processes with a high flexibility index are expected to be easier to control, while those with a low index will require good disturbance rejection if they are to be considered further. Disturbance rejection has also been examined by looking at the controllability of each process. The results of applying a step and an impulse disturbance to the feed of each process can be seen in section 7.3.8. Different results are obtained from the two analysis methods and therefore the flexibility and resilience results both have to be considered when determining the controllability of the process.

8.1.4 Multiple Objectives

With a large amount of data being made available to the designer it can be difficult to identify the issues which are important in the design. Multi-objective assessment methods have been proposed that help select the best processes, but the end result obtained is dependent upon the designers own personal preference and the information returned by the assessment tools. If the design set is large and quantifiable data is present then the most useful assessment method is statistical analysis of the data, which has been discussed in section 5.1.1. It can help to identify combinations of tests that produce the same result and can help spot relationships between tests. Outlying processes can be identified and the number of alternatives that need to be considered reduced.

Where one process is not immediately identified as being the best then an assessment based upon the designers values needs to be made. If the value between one measure and another is known then the analysis can be reduced to a single function. An example of this would be if the cost of introducing safety features into a process was known then the value of safety could be formulated. Unfortunately, this also requires that the relationship between tests is continuous, which is generally not true. For example, improving the safety of a plant usually requires the addition of individual safety equipment which give step changes in the safety index. Where discontinuous assessment exists lexicographical ordering can be used to help order the process alternatives. Lexicographical ordering has the advantage that the value function is simple, with one test being more desirable than another and a degree of tolerance in the results. This thesis has shown that by combining statistical analysis with the value based assessments the best process alternatives can be identified.

The ranking of the different ethylene processes is examined and shows that applying the multi-objective techniques can result in a different process ordering. Lexicographical ordering has been applied to the processes and places the most favourable process design as the seventh process from the original cost order.

With these tools the inherent benefits of different processes can be identified and brought forward for further design. As the information is improved then revisions can be made of past assumptions and the entire design space can be covered. The analysis requires the users input but should help steer the creativity of the design process to produce a successful process design.

8.2 Conclusions

We have developed a procedure for early consideration of multiple design criteria, which can help a designer to examine a number of design alternatives. The main features of the developed procedure is that the analysis is;

Flexible The analysis tools and databases are adjustable by the user, enabling the user to select the most appropriate information upon which to perform the analysis.

Extensible Further analysis tools can be added into the system.

Applicable The analysis tools developed are applicable to conceptual design.

Complementary The procedure fits into the design process from the point of generating conceptual designs to the point of developing detailed design.

Evaluation and analysis tools that evaluate the cost, safety, environmental impact, flexibility and controllability of a conceptual design have been developed along with multiple objective assessment methods to help find the best process alternative. This takes the design from the point of synthesis to a position where detailed design can be developed. The procedure has been demonstrated with hydrogen cyanide and ethylene case studies. It has been shown that the initial synthesis stage may not provide the best design, but the procedure developed can help the designer identify potential problems and provide the rational for selecting a smaller set of process alternatives.

Design is a decision making process and requires management of process information. This thesis uses an information management system that is capable of recording and analysing process data as the process is developed. This has enabled the strength and weaknesses of each process to be assessed early on in the design process.

The assessment tools have been chosen to be applicable to conceptual design and can progress as the process design is developed further. Being able to re-evaluate and perform a critical assessment of the decisions made is essential to maintaining confidence that the best process design has been chosen. Different techniques are used depending upon the assessment being performed. For example:

- Cost analysis utilises a spreadsheet format allowing the user to adjust cost factors and examine the sensitivity of each process.
- Safety and environmental assessments are carried out in self contained applications and return reports of the processes being examined.
- Flexibility and controllability analysis utilise the computation power of a mathematical package which enables the user to examine the response of the process.

Each of the assessment methods have been applied to a development case study which demonstrates the method and to two design case studies. The first case study analyses the production methods of hydrogen cyanide from an ammonia and methane feed. This case study has shown that the system is flexible enough to allow for revisions of the cost evaluation to be carried out. The costing analysis tool has shown how errors which were not obvious during the synthesis stage costing can be visualised and corrected. These corrections can be recorded in the management system so that the analysis can be returned back to the synthesis stage or the results corrected and the analysis taken forward. Controllability analysis shows how simplified models of the system can be generated, and their similarity to more detailed models used in the design process.

In the ethylene case study synthesis has been carried out on the separation section of the process. The synthesis stage returns a large number of process alternatives and identifying the most suitable alternative is not a simple task. A costing study shows that uncertainty in the operating and capital cost can affect the profitability of different alternatives along with changes to the economic climate. Safety analysis shows that there is a price to pay to achieve inherent safety. The controllability assessments demonstrate critical parts of each process and show where care must be taken when developing the control structure.

Multi-objective assessment methods have been proposed which can help the designer identify the critical information and rational the processes selected for detailed design.

The ethylene study has shown how this can be applied and how other conflicting objectives can be balanced. The assessment shows that the design selected upon a cost basis alone is not necessarily the best design and it would be desirable to take forward a smaller collection of processes for further design.

This thesis has shown the weakness of relying upon a single synthesis criterion and has demonstrated the benefits that can be gained by using a much broader design method. A flexible system of analysis has been proposed which can be extended to detailed design. By incorporating synthesis method into an environment that is informative the process alternatives can be assessed and the best designs taken forward for further consideration.

8.3 Recommendations For Future Work

This thesis has shown how a post synthesis design environment can be employed to help a designer assess and further develop conceptual designs. Because design is a broad subject there are many possibilities of extending the scope of applicability. Some recommendations which we believe would benefit the designer are as follows.

8.3.1 Adjustment of the Post Synthesis Tools to Cover a Wider Rage of Chemical Processes

The tools developed cover chemical processes which are continuous, vapour-liquid processes. Designers are likely to want to look at a much wider range of processes for example batch processes, solid processing or systems with complicated reaction-separation systems.

The needs of the designer determine the tools that will have to be developed, and their use requires maintenance of suitable database of the relevant extra information. Providing that the process the designer wishes to examine can be expressed in web objects the adjustment of the assessment tools should be possible.

8.3.2 Development of Further Analysis Tools

The tools developed show how the interconnections between parts of the process data is important in analysing the data. Further tools which assess the characteristics of the process can be developed such as plant silhouette, materials of construction, pressure relief etc.

The method has been created so that it can incorporate assessment tools which cover these situations. As mentioned in section 3 any tool which can assess a web object can be incorporated into the post synthesis analysis method.

8.3.3 Cyclic Process Synthesis

For each of the case studies the analysis has been performed on a single synthesis run. It would be desirable to incorporate optimisation tools across all design criteria into the analysis which adjust parameters of the search. This may give a different set of processes which can then be reanalysed. For example an optimisation analysis may adjust the feed stream to the process. As the feed stream is part of the original synthesis parameters the synthesis stage should be repeated with this new stream. The benefits of performing repeated synthesis this way should be examined.

8.3.4 Reverse Engineering

The procedure covers the design process from concept to the point of formulating a detailed design. It could be useful to examine existing processes which are usually a combination of design and evolution. It would be useful to know why they were designed the way they were. This would have the advantage that the trade off value between different criteria could then be explicitly evaluated and any inherent improvements to the system can be examined. The process of reverse engineering requires created a database of a large number of forwardly engineered processes and the decisions that were made in selecting the best process.

Bibliography

[1] J.E.Hendry D.F.Rudd. Synthesis in the design of chemical processes. *AIChE*, 19(1):1–15, 1973.

[2] L.T.Biegler I.E.Grossman A.W.Westerberg. *Systematic Methods of Chemical Process Design.* Prentice Hall, 1997.

[3] J.M.Douglas. *Conceptual Design of Chemical Processes.* McGraw Hill, 1 edition, 1988.

[4] D.F.Rudd. The synthesis of system designs, i: Elementary decomposition theory. *AIChE*, 14:343, 1968.

[5] M.M.Daichendt I.E.Grossmann. Integration of hierarchical decomposition and mathematical programming for the synthesis of process flowsheets. *Computers and Chemical Engineering*, 22(1):147–175, 1998.

[6] S.A.Papoulias I.E.Grossmann. A structural optimisation approach in process synthesis .1. utility systems. *Computers and Chemical Engineering*, 7(6):695–706, 1983.

[7] J.E.Hendry R.R.Hughes. Generating separation process flowsheets. *Chem. Eng. Prog.*, 19(1):1–15, 1972.

[8] W.R..Johns D.Romero. The automated generation and evaluation of process flowsheets. *Computers and Chemical Engineering*, 3:251–260, 1979.

[9] E.S.Fraga K.I.M.McKinnon. *CHiPS: A Process Synthesis Package*, 1993.

[10] M.D.Lu R.L.Motard. Computer-aided total flowsheet synthesis. *Computers and Chemical Engineering*, 9(5):431–445, 1985.

[11] I.E.Grossmann. Mixed-integer programming approach for the synthesis of integrated process flowsheets. *Computers and Chemical Engineering*, 9(5):463–482, 1985.

[12] M.A.Duran I.E.Grossmann. A mixed-integer nonlinear-programming algorithm for process systems synthesis. *AIChE Journal*, 32(4):592–606, 1986.

[13] C.A.Floudas A.R.Ciric I.E.Grossmann. Automatic synthesis of optimum heat-exchanger network configurations. *AIChE Journal*, 32(2):276–290, 1986.

[14] C.A.Flodas. Separation synthesis of multicomponent feed streams into multicomponent product streams. *AIChE Journal*, 33(4):540–550, 1987.

[15] G.R.Kocis I.E.Grossmann. Global optimisation of nonconvex mixed-integer nonlinear-programming (minlp) problems in process synthesis. *Industrial and Engineering Chemistry Research*, 27(8):1407–1421, 1988.

[16] J.Cerda AW.Westerberg D.Mason B.Linnhoff. Minimum utility usage in heat-exchanger network synthesis - a transportation problem. *chemical Engineering Science*, 38(3):373–387, 1983.

[17] M.A.Padley. *Incorporating Operability Measures into Process Synthesis.* PhD thesis, The University of Sydney, 1991.

[18] I.D.L.Bogle M.A.Steffans, E.S.Fraga. Multicriteria process synthesis for generating sustainable and economic bioprocesses. *Computers and Chemical Engineering*, 23:1455–1467, 1999.

[19] J.L.Robertson E.Subrahmanian M.E.Thomas A.W.Westerberg. Management of the design process: The impact of information modelling. *The 5th International Symposium on Process Systems Engineering*, pages 154–165, 1994.

[20] G.H.Ballinger R.Banares-Alcántara D.Costello E.S.Fraga J.Krabbe H.Lababidi D.M.Laing R.C.McKinnel J.W.Ponton N.Skilling M.W.Spenceley. épée: a process engineering software environment. *Computers and Chemical Engineering*, 18:S283–S287, 1994.

[21] R.Andrews J.W.Ponton. A process engineering information management system using world wide web technology. *FOCAPO. Utah*, 1998.

[22] R.McKelvey P.Piela A.Westerberg. An introduction to the ascend modelling system: Its language and interactive environment. *Journal of Management Information Systems*, 9:91–121, 1993.

[23] Eric S. Fraga. *CHiPS: A User's Manual.* The University of Edinburgh, Edinburgh, November 1994.

[24] M.S.Peters K.D.Timmerhaus. *Plant Design and Economics for Chemical Engineers.* Mc-Graw Hill, 4 edition, 1991.

[25] Aspen Technology, Inc, Cambridge, Massachusetts, USA. *Aspen Plus. Reference Manual-Volume 4.*

[26] K.M.Guthrie W.R.Grace. Data and techniques for preliminary capital costing. *Chemical Engineering*, 76:114–142, 1969.

[27] W.D.Baasel. *Preliminary Chemical Engineering Plant Design.* Elsevier, New York, 1976.

[28] A.Chauvel P.Leprince Y.Barthel C.Raimbautt J.Arlie. *Manual of Economic Analysis of Chemical Processes.* McGraw-Hill, 1 edition, 1976.

[29] J.Sweeting. *Project Cost Estimating - Principles and Practice.* IChemE, 1 edition, 1997.

[30] F.P.Lees. *Loss Prevention in the Process Industries*, volume 1. Butterworth-Heinemann Ltd, 1992.

[31] T.Kletz. *Plant Design for Safety: A User Friendly Approach.* Hemisphere publishing, 1991.

[32] AIChE, New York. *Guidelines for Hazard Evaluation Procedures*, 1992.

[33] T.A.Kletz. *Hazop and Hazan: Notes on the Identification and Assessment of Hazards.* IChemE, 1983.

[34] G.Wells. *Hazard Identification and Risk Assessment.* IChemE, 1996.

[35] CISHC (Chemical Industry Safety and Health Council). A guide to hazard and operability studies. Technical report, Chemical Industries Association, 1977.

[36] A.R.Bunn F.P.Lees. Expert design of plant handling hazardous materials. *Chemical Engineering Research and Design*, 66(5):419–444, 1988.

[37] A.Waters J.W.Ponton. Qualitative simulation and fault propagation in process plants. *Chemical Engineering Research and Design*, 67(4):407–422, 1989.

[38] A.Waters. *Knowledge Based Techniques in Plant Design for Safety*. PhD thesis, University of Edinburgh, 1991.

[39] AIChE, New York. *Dow Fire and Explosion Index. A Hazard Classification Guide*, 7 edition, 1994.

[40] D.J.Lewis. The mond fire, explosion and toxicity index: A development of the dow index. In *AIChE Loss Prevention Symposium*, Houston, 1979. AIChE.

[41] AIChE, New York. *Dow Chemical Exposure Index Guide*, 1 edition, 1994.

[42] AIHA Emergency Response Planning Committee. *Emergency Response Planning Guidelines Series*.

[43] M.M.Mumtaz K.A.Poirier J.T.Colman. Risk assessment for chemical mixtures: Fine-tuning the hazard index approach. *Journal of Clean Technology, Environmental Toxicology and Occupational Medicine*, 6:189–204, 1997.

[44] P.Sharratt. Environmental criteria in design. *Computers and Chemical Engineering*, 23:1469–1475, 1999.

[45] L.E.Wallin A.A.Metry. Lca - a tool for marketing clean products. *Journal of Clean Technology and Environmental Sciences*, 2(3):205–213, 1992.

[46] R.Zanetti. Lca - walk before you run. *Chemical Engineering*, 100(7):5, 1993.

[47] D.J.Brennan. Some challenges of cleaner production for process design. *Environmental Protection Bulletin*, 24:3–7, 1993.

[48] C.Krotscheck M.Narodoslawsky. The sustainable process index. a new dimension in ecological evaluation. *Ecological Engineering*, 6:241–258, 1996.

[49] R.Heijungs, editor. *Environmental Life Cycle Assessment of Products.* NOH, 1991.

[50] I.E.Grossmann K.P.Halemane R.E.Swaney. Optimisation strategies for flexible chemical processes. *Computers and Chemical Engineering*, 7:439, 1983.

[51] A.M.Lenhoff M.Morari. Design of resilient processing plants 1. process design under consideration of dynamic aspects. *Chemical Engineering Science*, pages 245–258, 1982.

[52] R.E.Swaney I.E.Grossmann. An index for operational flexibility in chemical process design: Formulation and theory. *AIChE Journal*, 31(4):621–630, April 1985.

[53] R.E.Swaney I.E.Grossmann. An index for operational flexibility in chemical process design: Computational algorithms. *AIChE Journal*, 31(4):631–641, April 1985.

[54] A.Brian M.Breiner. *Matlab for Engineers.* Addison-Wesley, 1997.

[55] M.Morari. Design of resilient processing plants-3. *Chemical Engineering Science*, 38:1881-1891, 1983.

[56] The Math Works Inc. *Control System Toolbox*, 1998.

[57] E.F.Wahl P.Harriott. Understanding and prediction of the dynamic behaviour of distillation columns. *Industrial and Engineering Chemistry Process Design and Development*, 9(3):396–407, 1970.

[58] Hyprotech Ltd., Calgary. *Hysys, Version 1.0 Reference*, 1 edition, 1995.

[59] M.Kendall. *Multivariate Analysis.* Charles Griffin and Company Ltd, 2 edition, 1980.

[60] R.L.Keeny H.Raiffa. *Decisions with Multiple Objectives:Preferences and Value Tradeoffs.* John Wiley and Sons Inc, 1 edition, 1976.

[61] J.L.Cohon. *Multiobjective Programming and Planning.* Academic Press, London, 1 edition, 1978.

[62] R.E.Kirk D.F.Othmer. *Encyclopedia of Chemical Technology*, volume 7. 4 edition, 1991.

[63] D.E.Seborg T.F.Edgar D.A.Mellichamp. *Process Dynamics and Control.* John Wiley and Sons Inc, New York, 1 edition, 1989.

[64] G.F.Froment. Thermal cracking for olefins production. fundamentals and their application to industrial problems. *Chemical Engineering Science*, 36:1271–1282, 1981.

[65] R.E.Kirk D.F.Othmer. *Encyclopedia of Chemical Technology*, volume 9. 4 edition, 1991.

[66] R.C.Reid J.M.Prausnitz P.B.Poliny. *The Properties of Gases and Liquids.* Mc Graw Hill, New York, 4 edition, 1987.

Appendix A

Glossary

A.0.5 Nomenclature

`Class` = Web object which contains processes which share a common feature.

`Control` = Web object describing relationship between transfer functions

`Domain` = Web object which contains all possible processes

$G(s)$ = Transfer function

$HAZAN$ = Hazard Analysis

$HAZOP$ = Hazard and Operability Studies

`Initialisation object` = Web object used to set synthesis settings

L_R = Reduced circulation rate

`Report` = Web object showing variable values and providing a link to results

`Unit` = Web object containing information about a unit

s = Laplace transform variable

`Statistics` = Web object containing extra information for `streams` and `units`

`Stream` = Web object containing information about a stream

`Task` = Web object defining a synthesis task

`Transfer` = Web object which contains transfer function information.

`Topology`= Web object describing relationship between streams and units

T_s = Model Time constant

X_p^n = Observation vector of sample n with length p

x_{np} = observation matrix of n samples and p tests.

Greek letters

α = Relative Volatility
θ = Test series
μ = Mean value
σ = Standard deviation

A.0.6 Abbreviations

AP = Acidification Potential
CEI = Chemical Exposure Index
CGI = Common Gateway Interface
ECA = Ecotoxicity Classification Aqueous
ECT = Ecotoxicity Classification Terrestrial
FEI = Fire and Explosion Index
GWP = Global Warming Potential
HCA = Human Toxicological Classification (Air)
HCS = Human Toxicological Classification (Soil)
HCW = Human Toxicological Classification (Water)
IRR = Internal Rate of Return
LCA = Life Cycle Assessment
$MILP$ = Mixed Integer Linear Program
$MIMO$ = Mixed Input Mixed Output
$MINLP$ = Mixed Integer Nonlinear program
MW = Molecular Weight
$M\&S$ = Marshall and Swift index
NP = Nutification Potential
NPV = Net Present Value
ODE = Ordinary Differential Equations
ODP = Ozone Depletion Potential
$P\&ID$ = Process and Instrumentation Diagram
$POCP$ = Photochemical Ozone Creation Potential

`SISO` = Single Input Single Output

WWW = World Wide Web

Appendix B

Safety Data

B.1 FEI Penalty Contributions

Toxic Materials. Toxic materials can reduce the ability of operators to take action in the case of an incident and incur a penalty of $0.2 * Nh$.

Sub-Atmospheric Pressure. Pressure less than 500 mm Hg incur a penalty of 0.5.

Operation In or Near Flammable Range. If $Nf >= 3$ A penalty of 0.5 is added.

Dust Explosion. Dust explosions are ignored in this analysis.

Relief Pressure. Relief pressure is assumed to be 25 % above operating pressure.

Low Temperature. To allow for brittle failure of steel processes operating below 10 °C incur a penalty of 0.3.

Quantity of Flammable/Unstable Material. Depending upon the amount of liquid/gases present in the process and storage results receive a penalty between 0.1 and 2.

Corrosion and Erosion. All processes suffer from corrosion and a base penalty is assumed at 0.1. For highly corrosive applications this should be increased up to 0.75.

Leakage. A base penalty factor of 0.1 is assumed for leaks from joints. This should be increased up to 1.5 if leaking equipment is used such as bellows or expansion joints.

Use of Fired Equipment. The addition of fired equipment increases the probability of an ignition source. The analysis assumes no fired equipment is present and no penalty is taken.

Hot Oil Heat Exchange. Assume no hot oil exchange therefore no penalty.

Rotating Equipment. Assume no rotating equipment therefore no penalty.

B.2 Damage Factor Coefficients

MF	Dfa	Dfb	Dfc	Dfd
< 1	0.0039	0.0030	0.0040	0.00029
1-4	0.028	0.019	0.00081	0.00011
4-10	0.099	0.018	0.00081	0.000013
10-14	0.21	0.019	0.0076	0.00057
14-16	0.26	0.020	0.011	0.00088
16-21	0.34	0.077	0.0039	0.00073
21-24	0.40	0.096	0.0014	0.00038
24-29	0.48	0.094	0.0022	0.00031
> 29	0.55	0.081	0.00033	0.00044

Table B.1: Damage Factor Coefficients

Appendix C

Control

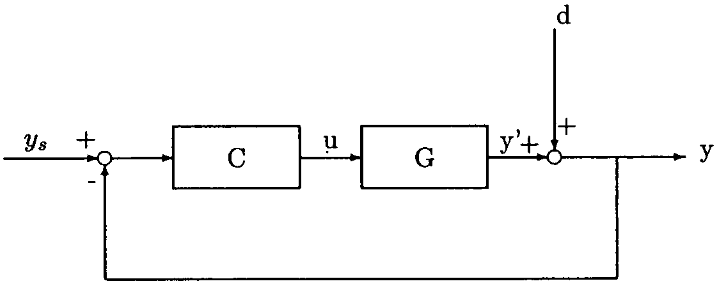


Figure C.1: A typical feedback control structure

The system is represented by the transfer matrix.

$$y(s) = G(s)u(s) \tag{C.1}$$

Where $y(s) \epsilon R^n$ are the outputs to be controlled and $u(s) \epsilon R^m$ are the manipulated variables. The system is represented by $G(s) \epsilon R^{n*m}$ and feedback represented by $C(s) \epsilon R^{m*n}$. $y_s \epsilon R^n$ are the set points for the system and $d \epsilon R^n$ are the disturbances.

Ideally the output matches the set point

$$y(t) = y_s(t) \tag{C.2}$$

Therefore the output from the system plus the disturbance match the set point

$$y_s(s) = y'(s) + d(s) \tag{C.3}$$

This then requires that

$$u(s) = G^{-1}(s)(y_s(s) - d(s)) \tag{C.4}$$

Where $G(s)G^{-1}(s) = I$. Providing that G^{-1} can be found then perfect control is possible.

Appendix D

Hydrogen Cyanide Case Study Data

Units refer to the processes in figres 6.1, 6.2 and 6.3.

D.1 Component Material Factors

Ammonia	4	3	1	0
Methane	21	1	4	0
Hydrogen Cyanide	24	4	4	2
Hydrogen	21	0	4	0

D.2 Fire and Explosion Results

Process 1 Fire and Explosion Index Results

	Mixer	Reactor	F1	T100
Dows FEI	1.6	1.99	1.83	1.98
Damage Factor	0.26	0.51	0.58	0.59

Process 2 Fire and Explosion Index Results

	Mixer	T100	Reactor	F1
Dows FEI	1.74	2.28	1.98	1.86
Damage Factor	0.33	0.54	0.51	0.58

Process 3 Fire and Explosion Index Results

	Mixer	Reactor	T100	F1
Dows FEI	1.62	1.99	1.91	1.80
Damage Factor	0.26	0.51	0.59	0.50

D.3 Chemical Exposure Results

Process 1 Chemical Exposure Results

	Feed	1	3	4	5	7	6
Exposure Index	3.52	3.58	2.22	2.12	2.42	13.7	2.57
Airborne Quantity	0.73	0.72	0.44	0.52	0.51	0.73	0.47
Hazard Distance	35.3	35.8	22.3	21.3	24.7	137.0	25.7

Process 2 Chemical Exposure Results

	Feed	1	2	3	5	7	8
Exposure Index	4.24	5.38	194.9	4.29	2.29	2.11	56.5
Airborne Quantity	1.05	1.15	1.03	1.05	0.46	0.51	0.86
Hazard Distance	42.4	53.8	10000	42.9	22.9	21.1	565.0

Process 3 Chemical Exposure Results

	Feed	1	3	4	5	6	7
Exposure Index	3.53	3.58	2.30	3.13	1.98	2.47	14.4
Airborne Quantity	0.73	0.73	0.46	0.70	0.44	0.62	0.81
Hazard Distance	35.3	35.8	23.0	31.3	19.8	24.7	144.0

Appendix E

Ethylene Case Study Data

E.1 Physical Property Data

Formula	TBP	PC	TC	VC	Δ HF	Δ GF	CpA	CpB	CpC	CpD
CH_4	111.6	46.0	463.4	0.099	-74.9	-50.9	1.93E1	5.21E-2	1.20E-5	-1.13E-8
C_2H_4	169.4	50.4	555.6	0.129	52.3	68.2	3.80	1.57E-1	-8.35E-5	1.76E-8
C_2H_6	184.5	48.8	578.6	0.148	-84.7	-33.0	5.40	1.78E-1	-6.94E-5	8.71E-9
C_2H_2	189.2	61.4	581.5	0.113	226.8	209.3	2.68E1	7.58E-2	-5.01E-5	1.41E-8
C_3H_8	231.1	42.5	643.0	0.203	-103.9	-23.5	1.84	3.49E-1	-2.24E-4	5.86E-8

Table E.1: Physical Property Data

TBP = Normal Boiling Point Temperature, K

PC = Critical Pressure, bar

TC = Critical Temperature, K

VC = Critical Volume, m^3/mol

$DelHF$ = Standard enthalpy of formation at 298K, KJ/mol

$DelGF$ = Standard Gibbs energy of formation at 298K, KJ/mol

CpA, CpB, CpC and CpD = Constants in the ideal gas equation.

$Cp = CpA + CpB * T + CpC * T^2 + CpD * T^3$

Cp J/mol K

Physical property data from Reid [66].

E.2 Component Statistic Data

Component	MF	Nh	Nf	Nr	ERPG2	Greenhouse Index
ethylene	24	1	4	2	50000	8
ethane	21	1	4	0	50000	7
acetylene	29	0	4	3	50000	8
methane	21	1	4	0	50000	10
propane	21	1	4	0	50000	3

Table E.2: Statistic Data

MF = Material Factor

Nh = NFPA Classification for toxic materials.

Nf = NFPA Classification for flammable materials.

Nr = NFPA Classification for reactive materials.

$ERPG2$ = Maximum airborne concentration that individuals can be exposed to for upto one hour.

$GreenhouseIndex$ = Material Contribution to the enhancement of the greehouse effect with respect to emissions of CO_2 .

Mf,Nh,Nf,Nr are contained in Dows Fire and Explosion Index [39]. Values of ERPG2 are from Dows Chemical Exposure Index Guide [41]. Greenhouse Index values are from [49].

E.3 Greenhouse Results

Process Stream	1	2	3	4	5	6	7	8	9	10
1	7.41	7.41	7.41	7.41	7.41	7.41	7.41	7.41	7.41	7.41
2	7.41	7.41	7.41	7.59	7.41	7.41	7.41	7.41	7.41	7.41
3	7.52	7.52	7.52	7.25	7.52	7.52	7.52	7.52	7.52	7.52
4	7.52	7.52	7.52	7.25	7.55	7.52	7.55	7.52	7.52	7.52
5	6.63	6.63	6.63	2.54	6.67	6.63	6.89	6.54	2.22	2.23
6	6.63	6.63	6.53	5.78	7.55	6.53	2.08	7.53	7.52	7.52
7	2.25	2.25	6.61	5.78	7.55	6.61	6.89	6.11	6.66	6.66
8	6.59	6.59	2.24	7.55	2.24	2.24	7.33	7.53	6.62	6.62

Table E.3: Greenhouse Index

E.4 Process Profiles

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	0.51	0.01	0.01	0.00	5.30
Ethane	40.00	0.40	39.60	39.20	0.40	0.40	0.00	0.40
Acetylene	5.50	0.00	5.50	0.05	5.45	5.40	0.05	0.11
Propane	4.00	0.00	4.00	0.00	4.00	0.04	3.96	0.04
Temp (K)	150.0	187.8	204.4	214.4	223.9	222.3	256.7	451.7
Press (atm)	30.0	10.0	10.0	30.0	30.0	22.8	22.8	22.8
Phase	Liq	Vap	Liq	Vap	Liq	Vap	Liq	Liq

	Unit			
	T101	T102	T103	R101
Height (m)	22.6	4.7	6.1	5.2
Diameter (m)	0.5	0.6	0.1	2.6
Press (atm)	10.0	30.0	22.8	22.8
No. of Stages	31	116	20	-
Reflux Ratio.	1.07	4.77	0.32	-

Table E.4: Ethylene Process 1 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	52.50	0.00	0.00	0.00	0.00	0.00	5.13
Ethane	40.00	0.40	39.60	39.20	0.40	0.40	0.00	0.40
Acetylene	5.50	0.00	5.50	0.05	5.45	5.24	0.21	0.10
Propane	4.00	0.00	4.00	0.00	4.00	0.16	3.84	0.16
Temp (K)	150.0	187.8	204.4	214.4	223.9	219.3	249.8	451.7
Press (atm)	30.0	10.0	10.0	30.0	30.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Vap	Liq	Liq	Liq	Liq

	Unit			
	T201	T202	T203	R201
Height(m)	22.6	74.7	13.1	5.2
Diameter (m)	0.5	0.6	0.1	2.6
Press (atm)	10.0	30	30	30
No. of Stages	31	116	15	-
Reflux Ratio.	1.07	4.77	0.3	-

Table E.5: Ethylene Process 2 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	0.51	0.01	5.35	5.35	0.00
Ethane	40.00	0.40	39.60	39.20	0.40	0.40	0.40	0.00
Acetylene	5.50	0.00	5.50	0.05	5.45	0.11	0.10	0.01
Propane	4.00	0.00	4.00	0.00	4.00	4.00	0.16	3.84
Temp (K)	150.0	187.8	204.5	214.4	223.9	451.7	197.8	231.1
Press (atm)	30.0	10.0	10.0	30.0	30.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Vap	Liq	Liq	Liq	Liq

	Unit			
	T301	T302	R301	T303
Height (m)	22.6	74.7	6.2	14.3
Diameter (m)	0.5	0.6	3.1	0.12
Press (atm)	10.0	30.0	30.0	30.0
No. of Stages	31	116	-	17
Reflux Ratio.	1.07	4.77	-	0.99

Table E.6: Ethylene Process 3 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	0.51	0.01	5.84	5.78	0.06
Ethane	40.00	0.04	39.96	39.96	0.00	39.96	0.40	39.56
Acetylene	5.50	0.00	5.50	5.44	0.06	0.11	0.00	0.11
Propane	4.00	0.00	4.00	0.04	3.96	0.04	0.00	0.04
Temp (K)	150.0	197.9	215.2	215.6	258.7	451.7	200.5	214.4
Press (atm)	30.0	30.0	30.0	26.9	26.9	26.8	30.0	30.0
Phase	Liq	Vap	Liq	Vap	Liq	Liq	Vap	Liq

	Unit			
	T401	T402	R401	T403
Height (m)	22.7	16.8	10.4	51.5
Diameter (m)	0.4	0.3	5.2	0.5
Press (atm)	30.0	26.9	26.9	30.0
No. of Stages	31	21	-	78
Reflux Ratio.	1.06	0.14	-	28.09

Table E.7: Ethylene Process 4 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	5.91	5.86	0.05	0.05	0.00
Ethane	40.00	0.40	39.60	39.60	0.40	39.20	39.20	0.00
Acetylene	5.50	0.00	5.50	0.11	0.11	0.00	0.00	0.00
Propane	4.00	0.00	4.00	4.00	0.00	4.00	0.04	3.96
Temp (K)	150.0	197.9	215.2	451.7	200.5	215.3	216.4	240.8
Press (atm)	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Liq	Vap	Liq	Vap	Liq

	Unit			
	T501	R501	T502	T503
Height (m)	22.7	10.7	51.5	15.8
Diameter (m)	0.4	5.4	0.5	0.3
Press (atm)	30.0	30.0	30.0	30.0
No. of Stages	31	-	78	19
Reflux Ratio.	1.06	-	28.69	0.14

Table E.8: Ethylene Process 5 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.53	0.52	0.01	5.35	5.35	0.00
Ethane	40.00	0.40	39.60	39.20	0.40	0.40	0.40	0.00
Acetylene	5.50	0.00	5.50	0.05	5.45	0.11	0.11	0.00
Propane	4.00	0.00	4.00	0.00	4.00	4.00	0.04	3.96
Temp (K)	150.0	187.8	204.4	214.4	223.9	451.7	220.0	248.0
Press (atm)	30.0	10.0	10.0	30.0	30.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Vap	Liq	Liq	Vap	Liq

	Unit			
	T601	T602	R601	T603
Height (m)	22.6	74.7	6.2	18.1
Diameter (m)	0.5	0.6	3.1	0.1
Press (atm)	10.0	30.0	30.0	30.0
No. of Stages	31	116	-	23
Reflux Ratio.	1.07	4.77	-	1.07

Table E.9: Ethylene Process 6 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	5.91	5.91	0.00	5.86	0.05
Ethane	40.00	0.40	39.60	39.60	39.60	0.00	0.40	39.20
Acetylene	5.50	0.00	5.50	0.11	0.11	0.00	0.00	0.11
Propane	4.00	0.00	4.00	4.00	0.04	3.96	0.00	0.04
Temp (K)	150.0	197.9	215.2	451.7	213.3	238.1	200.5	214.4
Press (atm)	30.0	30.0	30.0	30.0	24.1	24.1	30.0	30.0
Phase	Liq	Vap	Liq	Liq	Vap	Liq	Vap	Liq

	Unit			
	T701	R701	T702	T703
Height (m)	22.7	10.7	23.0	27.2
Diameter (m)	0.4	5.4	0.3	0.4
Press (atm)	30.0	30.0	24.1	30.0
No. of Stages	31	-	31	38
Reflux Ratio.	1.06	-	0.66	16.86

Table E.10: Ethylene Process 7 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	0.51	0.01	5.68	5.62	0.06
Ethane	40.00	0.40	39.60	39.60	0.00	39.60	0.40	39.20
Acetylene	5.50	0.00	5.50	5.28	0.22	0.11	0.00	0.11
Propane	4.00	0.00	4.00	0.16	3.84	0.16	0.00	0.16
Temp (K)	150.0	197.9	215.2	214.9	249.8	451.7	200.5	214.4
Press (atm)	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Liq	Liq	Liq	Vap	Liq

	Unit			
	T801	T802	R801	T803
Height (m)	22.7	13.9	10.4	51.5
Diameter (m)	0.4	0.3	5.2	0.5
Press (atm)	30.0	30.0	30.0	30.0
No. of Stages	31	16	-	78
Reflux Ratio.	1.06	0.11	-	28.09

Table E.11: Ethylene Process 8 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	0.51	0.01	0.51	0.00	5.13
Ethane	40.00	0.40	39.60	39.60	0.00	39.20	0.40	0.40
Acetylene	5.50	0.00	5.50	5.28	0.22	0.05	5.23	0.10
Propane	4.00	0.00	4.00	0.16	3.84	0.00	0.16	0.16
Temp (K)	150.0	197.9	215.2	204.2	236.8	214.4	218.6	451.7
Press (atm)	30.0	30.0	30.0	10.0	10.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Liq	Liq	Vap	Liq	Liq

	Unit			
	T901	T902	T903	R901
Height (m)	22.6	13.8	74.6	5.2
Diameter (m)	0.4	0.4	0.6	2.6
Press (atm)	30.0	10.0	30.0	30.0
No. of Stages	31	16	116	-
Reflux Ratio.	1.06	0.17	4.76	-

Table E.12: Ethylene Process 9 Profile

	Stream							
Kmol/hr	1	2	3	4	5	6	7	8
Ethylene	52.50	51.98	0.52	0.51	0.01	0.51	0.00	5.28
Ethane	40.00	0.40	39.60	39.60	0.00	39.20	0.40	0.40
Acetylene	5.50	0.00	5.50	5.44	0.06	0.05	5.39	0.11
Propane	4.00	0.00	4.00	0.04	3.96	0.00	0.04	0.04
Temp (K)	150.0	197.9	215.2	206.4	247.0	214.4	218.0	451.7
Press (atm)	30.0	30.0	30.0	10.0	10.0	30.0	30.0	30.0
Phase	Liq	Vap	Liq	Vap	Liq	Vap	Liq	Liq

	Unit			
	T1001	T1002	T1003	R1001
Height	22.6	16.8	75.3	5.2
Diameter	0.4	0.4	0.6	2.6
Press	30.0	10.0	30.0	30.0
No. of Stages	31	21	117	-
Reflux Ratio.	1.06	0.15	4.98	-

Table E.13: Ethylene Process 10 Profile

E.5 Control Constants

	T101	T102	T103	T201	T202	T203	T301	T302	T303	T401	T402	T403	T501	T502	T503
Ts	16.91	124.75	8.52	16.91	124.75	5.34	16.91	124.75	6.56	16.91	9.21	68.66	16.91	68.66	7.85
T1	15.57	121.87	0.64	15.57	121.83	0.10	15.57	121.87	4.06	15.52	6.78	62.20	15.57	62.22	5.50
T2	0.40	0.58	3.18	0.40	0.59	2.09	0.40	0.58	1.06	0.42	0.98	2.03	0.40	2.02	0.97
T3	0.52	5.30	1.75	0.52	5.38	0.98	0.52	5.30	1.19	0.54	0.16	97.98	0.52	99.59	0.15
T4	0.26	2.05	0.96	0.26	2.08	0.57	0.26	2.05	0.67	0.27	0.09	40.99	0.26	41.67	0.08
Tz	0.64	1.80	4.41	0.64	1.83	2.72	0.64	1.80	1.51	0.67	1.30	21.12	0.64	21.41	1.27

Table E.14: Time Constants Process 1-5

	T601	T602	T603	T701	T702	T703	T801	T802	T803	T901	T902	T903	T1001	T1002	T1003
Ts	16.91	124.75	10.63	16.91	16.91	23.10	16.91	5.94	68.66	16.91	5.94	124.75	16.91	9.21	126.37
T1	15.57	121.87	6.71	15.57	15.51	19.99	15.57	4.05	61.98	15.57	4.57	122.04	15.57	6.88	123.72
T2	0.40	0.58	1.66	0.40	0.42	1.08	0.40	0.79	2.12	0.40	0.54	0.54	0.40	0.93	0.52
T3	0.52	5.29	2.27	0.52	0.34	24.77	0.52	0.09	102.36	0.52	0.09	4.86	0.52	0.16	4.94
T4	0.26	2.05	1.21	0.26	0.17	11.97	0.26	0.05	42.83	0.26	0.05	1.88	0.26	0.09	1.91
Tz	0.64	1.80	2.58	0.64	0.64	6.14	0.64	1.00	22.06	0.64	0.68	1.65	0.64	1.24	1.64

Table E.15: Time Constants Process 6-10

	T101	T102	T103	T201	T202	T203	T301	T302	T303	T401	T402	T403	T501	T502	T503
Gxd	0.99	0.01	0.93	0.99	0.01	0.93	0.99	0.01	0.93	0.99	0.13	0.13	0.99	0.13	0.27
Gxb	0.20	0.96	Div/0	0.20	0.96	Div/0	0.20	0.96	Div/0	0.20	Div/0	0.27	0.20	0.91	Div/0
Grd	-0.99	0.01	-0.25	-0.99	0.01	-0.24	-0.99	0.01	0.62	-0.99	-0.03	0.13	-0.99	0.13	7.13
Grb	1.05	-95.40	Div/0	1.05	-95.40	Div/0	1.05	-95.40	Div/0	1.05	Div/0	-29.00	1.05	-91.09	Div/0
Gbd	0.99	0.00	0.00	0.99	0.00	0.00	0.99	0.00	0.00	0.99	0.00	0.00	0.99	0.00	0.00
Gbb	0.00	0.01	Div/0	0.00	0.01	Div/0	0.00	0.01	Div/0	0.00	Div/0	0.00	0.00	0.00	Div/0

Table E.16: Process Gains 1-5. For ethane concentarion with respect to disturbances in feed ethane concentration.

	T601	T602	T603	T701	T702	T703	T801	T802	T803	T901	T902	T903	T1001	T1002	T1003
Gxd	0.99	0.01	0.93	0.99	0.13	0.13	0.99	0.13	0.13	0.99	0.13	0.01	0.99	0.13	0.01
Gxb	0.20	0.96	Div/0	0.20	Div/0	0.27	0.20	Div/0	0.40	0.20	Div/0	0.93	0.20	Div/0	0.93
Grd	-0.99	0.01	0.66	-0.99	0.08	0.13	-0.99	-0.03	0.13	-0.99	-0.03	0.01	-0.99	-0.03	0.01
Grb	1.05	-95.40	Div/0	1.05	Div/0	-29.00	1.05	Div/0	-42.15	1.05	Div/0	-92.85	1.05	Div/0	-92.90
Gbd	0.99	0.00	0.00	0.99	0.00	0.00	0.99	0.00	0.00	0.99	0.00	0.00	0.99	0.00	0.00
Gbb	0.00	0.01	Div/0	0.00	Div/0	0.00	0.00	Div/0	0.00	0.00	Div/0	0.01	0.00	Div/0	0.01

Table E.17: Process Gains 6-10. For ethane conentration with respect to disturbances in feed ethane concentration.