THE MODELLING AND CONTROL OF A
1-OCTENE DIVIDING WALL
DISTILLATION COLUMN

Muhammad Abdul Kader, BSc Eng

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Date   **:**   August 2009
Supervisor   **:**   M. Mulholland

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ACKNOWLEDGEMENTS

ABSTRACT

Partitioned or Dividing Wall Columns (DWC) for distillation are currently receiving a lot more attention from industry because of their energy and capital cost reduction potential. These reductions occur due to the fact that only one column, reboiler and condenser are needed, as opposed to two complete conventional columns when a middle-cut is required.

A DWC has a vertical partition that divides the column shell into a prefractionator and a side draw section. The DWC and the Petlyuk column are thermodynamically identical, the difference between them being that the prefractionation section in a Petlyuk column is external and in a DWC it is contained within one shell. It is appropriate to model a DWC as a Petlyuk column when heat transfer effects across the wall are not significant. The purity of the middle product from a DWC is superior to that from a conventional side product column because the middle distillates usually form a strong split above and below the partition and the product is removed from the side of the partition remote from the feed.

The 1-octene prefractionator column on the SASOL Secunda site was investigated. Steady – state modelling is firstly undertaken in order to establish a model that matches the plant operating point. A first principles model was programmed using Microsoft Visual C++® while another stead-state model was developed using Aspen Plus® simulation software. The steady-state models matching the plant operating point were then converted to dynamic models so that unsteady-state testing could be performed around the operating point. The first principles model is programmed to evaluate a new set of conditions for the model in finite time intervals based on the previous set of conditions. The simulated Aspen Plus® model of the column was converted to a dynamic model utilising Aspen Dynamics®. The dynamic simulation was configured with the existing control scheme on the 1-Octene column. The purity of the Octene-rich side product was the major concern, so improvements of the control strategy were sought for more effective regulation of this composition.

The existing control scheme is made up of single input single output loops. Each measured input can only manipulate one output. The strong internal interactions and distributed nature of the column indicates that multiple relationships exist between variables. The column is thus a strong candidate for process control optimisation.

A 2x2 DMC controller was developed in Microsoft Visual C++® to better control the column. The controller was tested using both the first principles and simulated dynamic models.

Disturbance rejection is definitely improved using the advanced controller. Typical process perturbation sequences are applied, and set-point deviations evaluated, with a performance index being used to obtain best tuning.

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NOMENCLATURE

APC   Advanced Process Control

CV   Control Variable

DAE   Differential and Algebraic Equations

DOF   Degree of Freedom

DMC   Dynamic Matrix Control

DV   Disturbance Variable

DWC   Dividing Wall Column

LQG   Linear Quadratic Gaussian

LTR   Loop Transfer Rate

LQR   Linear Quadratic Regulator

MIMO   Multiple Input Multiple Output

MPC   Model Predictive Control

MV   Manipulated Variable

PID   Proportional Integral Derivative

P&ID   Piping and Instrumentation Diagram

PCES   Pure Component Equations of State

SISO   Single Input Single Output

A   Absorption Factor

S   Stripping Factor

M_i Overall Mass of components on tray i

N	Number of theoretical stages
Q_i	Heat addition/removal on tray i
F^L_n	Liquid to feed stage n
F^V_n	Vapour feed to stage n
h_n	Enthalpy of liquid leaving stage n
H_n	Enthalpy of vapour leaving stage n
h^{LF}_n	Enthalpy of liquid feed to stage n
H^{VF}_n	Enthalpy of vapour feed to stage n
h_{ow}	liquid height on weir
$K_{i,j}$	Equilibrium constant of component i on stage j
L_m	Liquid feed to stage n coming from remote stage m
L_n	Liquid flowrate leaving stage n
L_w	Weir Length
NC	Number of components
t	Time
U_n	liquid lateral extraction from stage n
$\bar{U}_n$	Internal energy of liquid retained on stage n
V_n	Vapour leaving stage n
W_n	vapour lateral stream drained from stage n
$X_{j,i}$	mol fraction of i in liquid phase leaving stage j
$Y_{j,i}$	mol fraction of i in vapour phase leaving stage j

$Z^{LF}_{n,i}$ mol fraction of i in liquid feed to stage n

$Z^{VF}_{n,i}$ mol fraction of i in vapour feed to stage n

1. INTRODUCTION

1.1   ORGANISATION OF THE THESIS

Chapter One: Introduction

This chapter gives an introduction and background to the Petroleum Industry and some of the methods used for separation of chemical mixtures. The process of distillation is briefly described without going into detail on the particular distillation technology used for this project. The chapter ends with a description of the background to the project.

Chapter Two: Energy Integrated Distillation Columns

This chapter delves into the background of energy integrated distillation columns. The theory and background with regards to dividing wall distillation columns is described.   Optimisation of the design of these columns is reviewed.

Chapter Three: Modelling of Dividing Wall Columns

The fundamentals of dividing wall columns are described in this chapter. The approach to modelling a column of this nature is investigated. Particular attention was given to the two methods of modelling undertaken in this study and they are described in more detail.

Chapter Four: Control of a Dividing Wall Column

Controllability analysis into the dividing wall column is described in this section. The chapter deals with regulatory control of the column. A complete controllability analysis is conducted on a dividing wall distillation column. Control system design is discussed from a theoretical standpoint. The control systems commonly found on dividing wall columns are reviewed and discussed with attention given to their pro's and cons and specifics with respect to the dynamics of a dividing wall column.

Chapter Five: Advanced Control

The techniques of advanced control are described in this chapter. The basic principles of advanced control are reviewed in particular detail. Other available industrial technologies for

advanced control are also described and discussed. The fundamentals on which the advanced controller was developed are reviewed.

Chapter Six: 1-Octene Model Development

The objectives of the model development is clearly discussed. A detailed description into the 1-Octene Column development and its topology, structure and mathematical solution are discussed. Features of the different models are also investigated.

Chapter Seven: Advanced Control of the 1-Octene Column

The strategy used for advanced control of the column is clearly discussed in this section of the column. Detailed descriptions are given with respect to the reasons for technology selection and implementation. The suitability of a controller of this nature is also described.

Chapter Eight: Discussion and Results

The project is briefly summarised and discussed before some of the results obtained from test simulations are analysed.

Chapter Nine: Conclusion

Conclusions about the modelling and control of the 1-Octene dividing wall distillation column are considered.

1.2   BACKGROUND TO PETROLEUM INDUSTRY

As the Industrial Revolution steamed along certain basic chemicals quickly became necessary to sustain growth. Sulfuric acid was the first chemical to be industrially produced.

In 1860 there were 15 refineries in operation. Known as "tea kettle" stills, they consisted of a large iron drum and a long tube which acted as a condenser. Capacity of these stills ranged from 1 to 100 barrels a day. A coal fire heated the drum, and three fractions were obtained during the distillation process. The first component to boil off was the highly volatile naphtha. Next came the kerosene, or "lamp oil", and lastly came the heavy oils and tar which were simply left in the bottom of the drum. These early refineries produced about 75% kerosene, which could be sold for high profits.

However, the naphtha and tar fractions were seen as valueless and were simply dumped. Later these waste streams were converted into valuable products. In 1869 Robert Chesebrough discovered how to make petroleum jelly and called his new product Vaseline. The heavy components began being used as lubricants, or as waxes in candles and chewing gum. Tar was used as a roofing material. But the more volatile components were still without much value. Limited success came in using gasoline as a local anesthetic and liquid petroleum gas (LPG) in a compression cycle to make ice. However, the general success in refined petroleum products greatly spread distillation. By 1865 there were 194 refineries in operation.

Petroleum refineries are marvels of modern engineering. Within them a maze of pipes, distillation columns, and chemical reactors turn crude oil into valuable products. Large refineries cost billions of dollars, employ several thousand workers and operate around the clock. The increase in industry capacity globally and the increase in the number of producers has resulted in a large excess capacity reducing profitability.

The refining industry is currently facing a difficult situation, characterized by decreasing profit margins, due to surplus refining capacity, and increasing oil prices. Simultaneously market competition and stringent environmental regulations are forcing the industry to perform extensive modifications in its operations. As a result, there is no refiner nowadays that does not use advanced process engineering tools to improve business results. Such tools range from advanced process control up to corporate long-term planning, passing through process optimization, scheduling, and short-term planning.

It is also worth mentioning that, due to pressure for cost reduction and the misguided view that automation should indiscriminately lead to staff reduction, most refiners do not possess enough experienced and trained engineering manpower to implement new process optimisation tools or even to maintain the existing ones. This has created a contradictory situation in which the benefits of advanced process technologies are widely recognised, but insufficient resources are available to keep them adequately operating and to develop and install new ones.

1.3 BACKGROUND TO THE PROJECT

The petrochemical industry is a technology driven industry which is why there is constant research being carried out in order to maintain the competitiveness and growth of the industry. In the year 1950 SASOL's first synthetic fuels plant was constructed in Sasolburg. The company has flourished since it's inception due to its continuous improvement with respect to technology as well as business acumen. The OPEC crisis in the early seventies presented the company with an opportunity to make a huge leap forward with the construction of their Secunda complex. The Secunda Complex is many folds larger than the Sasolburg plant, and produces a whole spectrum of products. SASOL became a private sector company in the year 1979 and had fully paid back the government by 1996; they are now listed on the international stock exchange and have many more business activities within and beyond the South African borders.

The main advantage that the unique SASOL Fischer-Tropsch process has is that it allows speciality chemicals to be produced at fuel prices. The main aim of SASOL was to produce fuel for South Africa from a non crude feedstock, yet the company now earns most of its income from other chemicals.

Longer chain alpha-olefins like 1-Octene have many uses such as their use as a co-monomer in the production of low-density polyethylene. 1-Octene has a high market value with an excellent potential for growth in the international market. The unique high temperature Fischer-Tropsch technology that is used by SASOL in their coal to oil process produces excellent straight chained olefin feedstock. This puts the company in an ideal position to play a strong role in this competitive part of the market. The company has been coming up with new ideas and optimising existing technology in order to increase their current production capacity of 1-Octene.

The 1-Octene train of separation processes was commissioned in 1998 with a capacity of approximately 50 000 tons per year. The continued growth of this sector of the market has led SASOL to develop and improve their technology as well as incorporate plans for the construction of an additional train in order to increase their market share in this sector. Optimisation of the current operating process and increasing the production efficiency of the 1-Octene train is highly important in order to maintain SASOL's position as one of the leaders in this field.

1.4 METHODS OF SEPARATION

Separation processes have been around for centuries. Some examples of early separation processes include the extraction of metals from ores, perfumes from flowers, dyes from plants, evaporation of sea water to obtain salt, and distilling of liquors. The human body also displays complex separations, one of them being the kidney which is a membrane that selectively removes water and waste products of metabolism from the blood.

There are two major categories in the realm of separation technology. One of them being mechanical separations e.g. filtration and the other involving changes in the properties of the solution which is referred to as a mass transfer operation. There also exist choices within mass transfer operations some of which being absorption, adsorption, distillation or liquid-liquid extraction as noted by R.P Williams (2003).

Most materials occur as mixtures of different components in either the gas, liquid or solid phase. In order to separate one or more of these components from the mixture it must be contacted with another phase which may include the introduction of energy into the system. When these two phases of the mixture are contacted the components of the original mixture redistributes itself between the two phases. One phase is enriched with certain components while the other is depleted of these components. The phases are separated from one another by physical methods. Methods of separation usually associated with chemical engineering involve the manufacture of chemicals using economical, large scale separation methods, which sometimes differs from the methods used in laboratories.

The key uses of separation on a chemical plant would be to purify raw materials, intermediates and products to the appropriate specification. Separations are achieved by enhancing the rate of mass transfer by diffusion of certain species relative to mass transfer of all species that remain in the bulk of that particular phase. The two crucial considerations that need to be taken into account are thermodynamics and transport operations. Many factors need to be taken into consideration before the appropriate method is chosen that would best suit the particular mixture, the solution of which sometimes lies in a process being developed that is a combination of more than one basic separation process.

The success of any separation process is based on the recovery and purity of the products. Although many different separation processes may be able to conduct the appropriate separation, it is usually the most technologically mature processes that are selected for

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commercial use. Ultimately the process having the lowest operating, maintenance and capital costs is selected.

1.5 DISTILLATION

"As we move through the 1980's, with full recognition of the energy intensiveness of distillation, we can expect to see relatively little displacement of distillation by alternative separation methods, at least for the large scale process throughputs. Thus, development of distillation devices will continue. The result will be improved separation efficiency at lower pressure drop and lower cost." Dr. James R. Fair, 1983

Distillation is a form of separation that has been around for thousands of years. The primary use of distillation in those times was to concentrate the alcohol content in beverages. The equipment used for distillation has vastly changed over the centuries, with the first vertical column being developed in 1813 in France by Cellier-Blumenthal. It was just after this that the initial idea of packings, bubble cap and sieve trays were developed. The first book on the topic of distillation was *La Rectification de l'alcohol* by Ernest Sorel in 1893.

At the dawn of the twentieth century distillation quickly transformed itself from just a tool for enhancing alcohol content in beverages to the prime method of separation in the chemical industry. The popularity of distillation in the chemical industry quickly escalated once it was recognised that distillation was an effective tool to separate crude oil into various products.

It is a method of separating components of a solution which depends upon the distribution of the substances between a vapour and liquid phase. The vapour or liquid phase is not added to the original mixture but it is formed from it by the addition of energy in the form of heat or work. The components of the mixture have different volatilities so that they will partition between the two phases to a different extent. If the differences in volatilities of the components are extremely small then separation will be extremely difficult and the process of distillation will in this case be uneconomical, and if the difference in volatilities of the components in the mixture are very large then the separation may be carried out in a single stage hence a flash separation may be carried out.
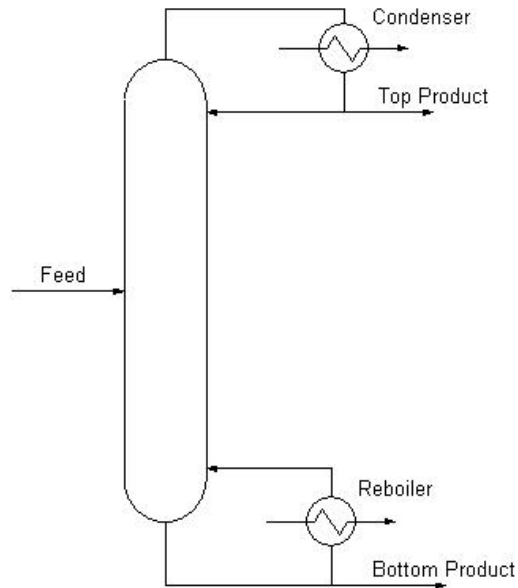
Figure 1.1 Conventional Distillation Column

A conventional distillation column as depicted in figure 1.1 contains one feed stream and two product streams. The top product stream is enriched with the lighter components and the bottom product stream is enriched with the heavier components. The column essentially contains two sections. The section above the feed stage is referred to as the rectification section and the section below the feed is called the stripping section. The top product vapour stream from the column passes through a condenser which can be a partial or total condenser, this provides liquid reflux that is fed back into the column, and the bottom liquid product is circulated through a partial reboiler which provides the energy input for the column.

In multicomponent distillation the terms simple and sharp separations are widely used. Simple separation is used when the feed is separated into two product streams and sharp being when a particular component entering in the feed stream leaves only in one of the product streams.

1.6   OBJECTIVES OF THE THESIS

The work in this thesis focuses primarily on the 1-Octene dividing wall distillation column located in Secunda, South Africa. This is a relatively new processing technology and as such there is a limited understand of the process. The dividing wall column technology also has a limited amount of industrial installations worldwide which makes it difficult to obtain knowledge from other users.

The development of first principle models to represent the process increases the fundamental understanding of the process. The models can then be converted to dynamic models and used to predict plant behaviour and hence conduct optimisation studies. The column itself is highly coupled making it difficult to operate and control. Existing regulatory control structures are investigated and advanced control technology developed in order to control the column.

Control studies are currently done on live plants and not using simulations because dynamic simulation is still a young technology. Steady-state simulations are not of much use because control has to do with the transient behaviour of the process as it moves from one steady-state to another. This study proves that dynamic simulation can be used as a tool to accurately test control configurations and advanced controllers.

2. ENERGY INTEGRATED DISTILLATION COLUMNS

2.1 INTRODUCTION

Distillation is certainly the most widely applied separation process and will continue to be an important process for the foreseeable future because there is currently no other industrially viable alternative. As research goes on for a better alternative, the process of distillation has also been improving. Breakthroughs have been made from time to time which has increased the level of sophistication of this process, yet it still remains one of the most energy intensive processes and operates with the lowest efficiency. Extensive research is still being carried out in order to reduce the energy consumption of this process.

For many years design engineers have had to face the problem of selecting the least expensive distillation sequence for separating multicomponent mixtures. The main reason for the great efficiency losses in distillation is that work is lost by heat transfer. This arises due to inefficient coupling of the heat sources and sinks as well as inefficient exchanges of heat and work with the environment. In a distillation sequence it is possible for the condenser of one column to provide some or all the heating required in the reboiler of another column operating at a lower temperature. If this type of heat integration between columns is allowed, the separation sequence synthesis problem is much more difficult because not only must the best distillation sequence be chosen, but the column pressures and heat exchanger network must be specified. Ways to help curb the energy intensity of distillation have been published with numerous variations to conventional distillation being carried out by S.P. Senda (2000). The main problem that is being addressed in this field is how to find the least expensive configuration of distillation columns which separates a given multicomponent mixture into a set of desired products.

The initial concepts behind the dividing wall distillation column can be traced back to the 1930's and 1940's with the US Patents of D. A. Monro (1946) and R. O. Wright (1946). At around the same time A. J. Brugma (1942) was laying the foundation of what is today known as thermally coupled distillation. The potential of these ideas were fully recognised by A. F. Petlyuk (1965) who published the article "*Thermodynamically Optimal Method for Separating Multicomponent Mixtures*" that represents the first major milestone in the development of this technology.

The research in this field had remained relatively dormant ever since the initial ideas surfaced, and only in the last ten years has the interest resurfaced. The limited energy reserves

remaining in the world and the constantly increasing price of energy have led to the continuation of this research. The Dividing Wall Column is now no longer just an academic concept with many installations worldwide as indicated by N. Hallale (2001). Many columns are currently in operation including two at SASOL in the 1-Hexene and 1-Octene plants. Distillation, being an integral process on most chemical plants with its energy intensive nature, makes the need for energy optimisation in distillation crucial in the current competitive market.

2.2   COMPLEX DISTILLATION

Good plant design ensures that there is minimum waste produced and a minimum amount of utilities consumed during operation. A complex distillation column arrangement involves columns with multiple feed and side stream products. These arrangements might have column sections with or without a reboiler or a condenser. Thermal coupling of two or more columns usually eliminates a reboiler or condenser by interchanging a liquid or vapour stream between the columns or column sections. A greater degree of separation is also achieved due to thermal coupling between the column sections.

Many different complex column arrangements may be used in order to achieve a separation, depending on a whole host of variables including the pressure and temperature under which the separation is to take place. Once all considerations have been taken into account, certain trade-offs need to be made in order to achieve an optimum design. The most important factors that affect the design of the separation process are operability, controllability and flexibility.

Some of the different column sequences described by Petlyuk and Platonov (1964) that may be used when trying to achieve a certain separation are expounded upon below:

Direct Sequence:
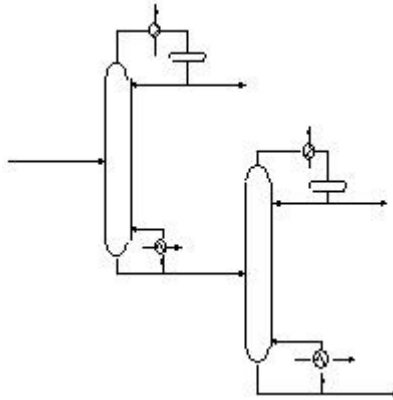
Figure 2.1 Direct Column Sequence

The sequence represented in figure 2.1 is used when the feed has a high concentration of the lightest components or when the separation of the middle distillate and the heavy product is slightly more difficult than that of the light and middle distillate. The light component is taken off as a distillate and the rest of the product is sent to a second column to undertake the subsequent separation. The columns are separated by a single liquid stream so they may be operated at different pressures in order to perform the optimum separation.

Indirect Column Sequence:
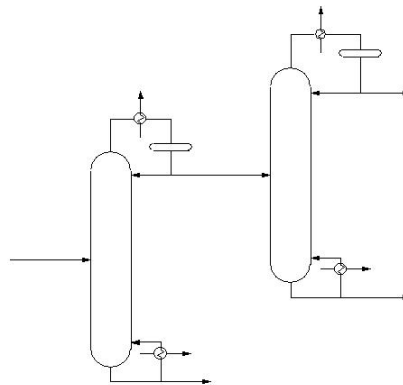
Figure 2.2 Indirect Column Sequence

This arrangement is most often used when the feed has a high concentration of the heavy product or when the separation of the light from the middle distillate is relatively more cumbersome. The heavy product is first separated out then the distillate is fed to a second column for further separation. For the vapour from a partial condenser the pressure in the second column needs to be lower than that of the first column for natural flow of the vapour, else a compressor would be needed between the columns. If a total condenser were used then the pressures in each column can be treated and optimised independently.

Distributed Column Sequence:
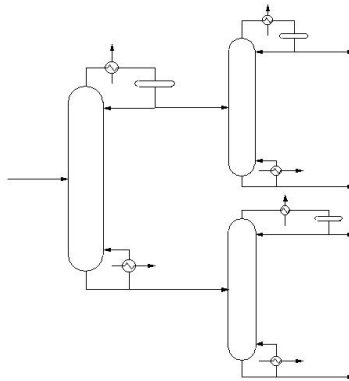
Figure 2.3 Distributed Column Sequence

This capital intensive arrangement requires three columns. It is considered most often when the required light, heavy and middle products are all close boiling materials and the separation can be done at low temperatures using lower quality utilities. This arrangement would also be considered when there is a high concentration of middle distillates in the feed. This configuration separates out the entire light component in the tops of the first column and the entire heavy product in the bottoms with the middle distillates being split between both these streams. The two subsequent columns separate light from middle and middle from heavy products.

Side Rectifier:
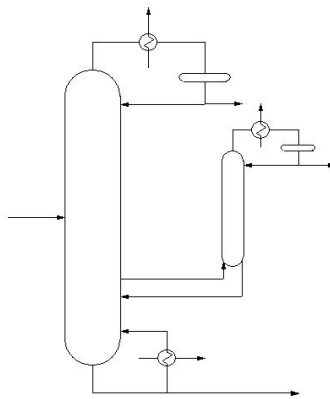
Figure 2.4 The Side Rectifier

A rectifier is thermally linked to the main column. This coupled column uses one reboiler to generate the vapour for both the columns but two condensers for liquid rectification. The entire system has to operate at the same pressure, but the pressure in the main column is slightly higher than that in the rectifier to accommodate for the natural flow of vapour.

A system similar to the Side Rectifier would be the Side Stripper. The difference being that in this arrangement there are two reboilers and only one condenser. In this case the stripping section operates at a slightly higher pressure for natural vapour flow to occur.

Pre-Fractionator:
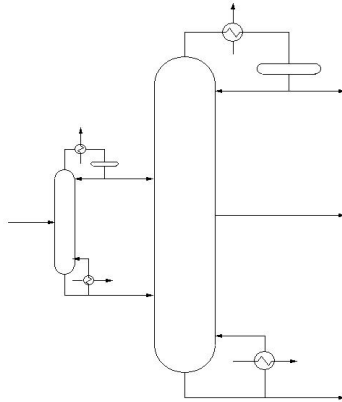
Figure 2.5 Pre-Fractionator

This configuration splits the feed into two feeds for the second column that has a side- draw as well. There are some similarities between this arrangement and the distributed sequence. This configuration can be thought of a coupling of the distributed arrangement and the removal of a condenser and a reboiler. This strategy is preferred when there is a large amount of middle distillate in the feed or it the splits between all fractions in the feed are difficult. Both columns may operate at different pressures in order to take advantage of utilities available at different temperatures for the Pre-Fractionator and Main column sections.

The Petlyuk Configuration:
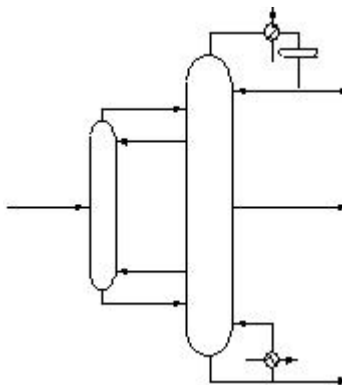
Figure 2.6 The Petlyuk Configuration

The Petlyuk configuration represents an arrangement that can separate three or more components using a single reboiler and a single condenser. This configuration has even more thermal coupling than the Pre-Fractionator which increases efficiency; this also means that there are greater internal flows with no hold-ups due to not having an intermediate reboiler or condenser in the Petlyuk column. The exchange of vapour and liquid between the columns poses strict pressure and operability constraints.

The Dividing Wall Column:
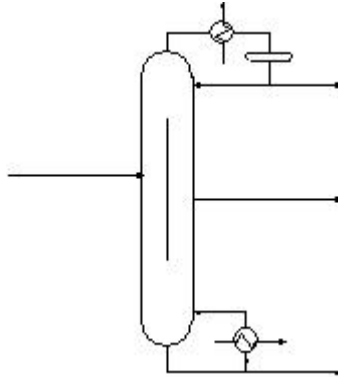
Figure 2.7 The Dividing Wall Column (DWC)

The dividing wall column represents the most compact configuration and allows for both considerable energy and capital saving. There is a partition between the feed and side-draw sections of the column which provides greater capacity and increased separation efficiency yet still externally resembles a normal side-draw column. This column is thermodynamically identical to the Petlyuk column provided that there is negligible heat transfer across the dividing wall of the column.

2.3   PETLYUK AND DIVIDING WALL COLUMNS

Finding the optimum arrangement with respect to column configuration and all other associated variables, can pose a complex mathematical problem which needs to be solved using rigorous mathematical procedures. In order to decrease the number of units used and the cost of separation, it is at times feasible to consider coupling column sections in order to reduce cost. The potential of using a conventional distillation column that has a side-draw is unattractive due to the fact that the products taken off as side-streams are never completely pure. When a side-stream is taken off in the rectification section of the column the product usually contains a certain amount of lower boiling materials which were to be taken out in the distillate and when a side-draw is taken in the stripping section of the column then the product usually contains a

proportion of higher boiling material that would have been removed in the bottom product. It is thus preferable only to use a conventional side draw column when impure side-stream products are permissible.

Most literature sources claim that the savings in both capital and energy costs when using a dividing wall column is in the region of 30% as compared to conventional arrangements using regular column sequences, and Glinos and Malone (1984) have concluded research that would indicate that the maximum savings are as large as 50%. Some of the arrangements, although complex, can be incorporated into one shell by using different types of dividing wall columns and more than one side stream. The pre-fractionation of feed on one side of the wall minimises the mixing losses while the thermal coupling that exists improves effective stripping and rectifying ratios. More than one partition could have an effect on the fabrication of trays as in the case of a column with two partitions and three sections. There are a large number of degrees of freedom for these complex arrangements, and all the variables need to be dealt with such that the operability challenges may be confronted.

Utilisation of the dividing wall column enables at least two conventional distillation columns to be replaced by a single dividing wall column. Several separations may be carried out in a single column using direct coupling of heat flows. The feed side of the column is separated and partitioned from the side draw part of the column. The feed is separated initially on this side of the column with the light and middle distillate components going up the column and the heavy and middle boiling material going down the column. Once the light and middle boiling components go above the partition the middle boiling material flows down on the other side of the partition sometimes using the method of adding an extra reflux to the column and the light components get taken out in the tops. The heavy and middle boiling material flow down to below the partition and the vapour rich in middle boiling distillate can flow up on the other side of the partition. The heavy material is taken out in the bottoms and the middle distillate rich stream is taken out as a side draw from the column. In a very similar way more than one dividing wall may be put into a column in order to increase the number of products drawn from the column. There is also a definite decrease in energy usage in these columns because all of the heat (boil-up) is supplied in the bottoms of the Petlyuk column and all of the cooling is carried out at the top of the column. The disadvantage of this may be the fact that the Petlyuk arrangement needs all the heat to be provided at the highest temperature and the cooling done at the lowest temperature, thus the cost of utilities may be more expensive as compared to configurations like the Pre-Fractionator that would require utilities at intermediate temperatures as well. When

dealing with close boiling materials it should be noted that a large number of stages may be required for this type of column and so pressure drop should also be considered closely. The dividing wall column is considered today to be an established technology with a steadily growing application potential in the petrochemical industry as indicated by N. Hallale (2001).

Based on the complex principles involved in dividing wall columns, there have been many methods proposed in order to optimise the design of such columns.

2.3.1   ENERGY SAVINGS

Finding ways to achieve minimum energy input has always been of interest. The initial work done by Underwood (1948) uses a rigorous iterative method based on the solution of the material balance equations corresponding to infinite columns. The next evolutionary step was taken by Petlyuk and Platonov (1964) who published a series of papers on the subject of a thermodynamically optimal distillation scheme. The methods used by these authors have laid the foundation and can be used as guidelines when trying to analyse real columns.

It has been shown by Malone (1985) that the relative costs of certain distillation sequences can be compared based on the total vapour requirements of that column. His findings imply that the column cross-sectional area and utility loads dominate the costs of the separation and that the effect of the number of stages is minimal in comparison provided that pressures are not extremely high and that corrosive components are not used.

More recently Fidkowski and Krolikowski (1986) completed a comprehensive analysis of the Underwood equations and have published that it is possible to recover the intermediate components of a mixture in a region of constant minimum energy. For most mixtures it has been found that it is optimum in terms of boil-up to use a vapour feed to the column. A degree of freedom analysis has been carried out by S. Skogestad (1992) and his findings indicate that there are five degrees of freedom in a Petlyuk column. In most cases three of these degrees of freedom are eliminated when product purity is set on each product stream. They had initially proposed that the two remaining degrees of freedom be used in order to control one of the impurities in the side product stream and the other to minimise energy consumption. It had later been proved by Morud (1995) that it is only possible to control the component purity of one component in each product stream from a Petlyuk Column.

It has been proved by S. Skogestad (1997) that the Petlyuk column is flexible because optimal operation is rather insensitive to disturbances when the column is running with a sharp separation. The Petlyuk column also contains a region in which the minimum vapour boil-up is constant which means that it may be operated over a range of recoveries without increasing the energy input to the column. The split of the rising vapour is very difficult to control and thus needs to be properly considered when designing the column such that it may be operated at all times within the optimal region.

On-going research in this field has led to new ideas being developed in order to optimise the energy consumption of these columns. The Infinite Dimensional State Space method Drake and Manousiouthakis (2000) is one such method that illustrates a rigorous mathematical method of carrying out this optimisation. It is based on a detailed process network diagram being constructed for the column that links all the major phenomena taking place within the column.

2.3.2   LEAST COST ALGORITHMS

This method is based on comparing all of the possible distillation arrangements that may be able to perform a particular separation and then selecting the arrangement that uses the least amount of utilities. The initial phase of this method requires all possible sequences to be identified. The next step is to approximate the capital and operating costs of those sequences using short cut methods. The minimum utility required for each sequence is then computed. It has also been noted that the sequence with the smallest utility demand and the sequence with the lowest number of columns will not occur on the same configuration. Based on this knowledge the optimum sequence needs to be selected. The optimum sequence is the sequence from among these that corresponds to the minimum cost. In this method it should also be noted that the column cost is calculated independent of column pressure. Columns that operate at elevated pressures require much thicker walled vessels. This means that over small and medium pressure ranges there are no significant errors in the computation, but as the pressure range gets large, the error in calculation could be quite significant. One of the ways of reducing this problem as suggested by Wenzel and Rohm (2004) is to introduce a ranking system based on volatility that will enable each column section to be calculated separately.

2.3.3 HEAT TRANSFER ACROSS THE WALL

Many literature sources including Traintafyllou and Smith (1992) and Wolff and Skogestad (1994) state that a dividing wall column is thermodynamically identical to a Petlyuk column provided that the heat transfer across the wall is negligible. At certain heights in the column there is a temperature gradient on either side of the wall which would cause some heat transfer horizontally across the wall. It is thus imperative to identify the portions of the wall at which heat transfer has any advantageous and ill effects. The appropriate portions of the wall will then need to be identified and proper action will be taken in order to solve the problem.

A number of simulations were carried out by Lestak (1994) in order to analyse the effect of heat transfer across the wall. The results show that heat transfer has a distinct effect on the duty required from the reboiler. It is thus imperative that this phenomenon be taken into account when designing Dividing Wall Columns.

The way in which this problem can be approached is to construct grand composite curves for the column that is being designed as shown by R. Smith (2000). These curves indicate the pinch points that exist in the column. This curve can be used to identify the portions of the column in which heat transfer across the wall is assisting the separation and zones in which the separation is being limited. These zones can then be designed with insulation in order to alleviate the detrimental effects of heat transfer. The tests should be repeated at different operating conditions such that sufficient insulation is installed. The optimisation of this aspect of the dividing wall column can translate to utility savings in the region of ten percent as suggested by Suphanit, Bischert and Narataruksa (2004).

2.3.4 DESIGN AND OPTIMISATION OF DIVIDING WALL COLUMNS

The task of simulating dividing wall columns has been extremely difficult due to the large number of variables that are involved. One of the approaches to designing a dividing wall column is to first develop a short-cut design procedure in order to assess the alternative designs that may be possible and perform preliminary optimisation. This can then be used as a starting point in order to perform a rigorous simulation.

The use of a NLP optimisation scheme is extremely cumbersome due to the numerous dependencies that are associated with the separation as well as the fact that the simulation may enter into an unstable region from which it cannot recover. A possibility that does exist in these

situations is the use of both a simulator and a MINLP optimisation routine provided that the simulation engine used is capable of combining these methods.

One of the methods suggested by Noronha and Gruhn (1997) that one can adapt and use to design a dividing wall column is based on calculating the number of stages needed as well as taking into account the way in which vapour flow will travel through the column. It is different to other methods that involve specifying the number of stages and predicting how they will perform. In order to perform this task, however, certain assumptions need to be made.

The procedure suggested by Stupin (1980) deals with both the vapour flow and the number of plates in each section of a Petlyuk column. The method however, is only applicable to ternary mixtures and does not deal in detail with flows to and from the pre-fractionator section to the main column

A system of short-cut equations was developed by Cerda and Westerberg (1979) which encompassed a whole range of distillation arrangements including the fully thermally coupled Petlyuk column. This method is only valid for sharp separations where the light and heavy key components do not occur in the bottom and top sections of the column respectively. Initial guesses are required for the minimum reflux ratio and the way in which components are spilt between the key components. The method for calculating the number of theoretical plates in the column is based on the method of using absorption factors by Edminster (1946). While this method for calculating the minimum reflux ratio has not been proven to be more accurate than the method of Underwood, it is considerably more complex than the Underwood method.

  A way in which to minimise vapour flow through the column under conditions of minimum reflux was developed by Fidkowski and Krolikowski (1986). The conditions that support their findings includes dealing with a ternary mixture, sharp separations, and a saturated liquid feed. The method does not include the number of theoretical stages which indicates that a rigorous simulation cannot be initiated based on the results of these findings.

The work of Glinos and Malone (1988) shows that the amount of vapour needed to run the column is independent of the vapour fed into the pre-fractionator provided that the side draw section of the main column remains unchanged. Their work is also based on a ternary mixture and the occurrence of a sharp separation. The result of this work reveals that there are infinite solutions for the amount of vapour fed to the pre-fractionator and the distribution of the middle key in the pre-fractionator.

Multicomponent mixtures with more than one middle key in the pre-fractionator were studied by Carlberg and Westerberg (1989) who carried out a detailed analysis of a fully thermally coupled column in terms of vapour flow. The formula utilised was the same as that used by Stupin (1980) however in this study the recovery of middle key components in the pre-fractionator is not considered an independent variable, but is dependant on the type of split and the recoveries obtained of the light and heavy key components.

Alatiqi and Luyben (1986) believed that the overall minimum vapour at minimum reflux is independent of the type of split and recoveries in the pre-fractionator. This has since changed, with the current belief being that the vapour flow in the main column is not independent of the vapour flow fed into the pre-fractionator. The separation is achieved even with the fluctuations in vapour and liquid draw-off rates at minimum vapour and minimum reflux conditions. It is thus imperative that the draw-off rates be optimised in order to accomplish the minimum energy requirement for a set number of stages.
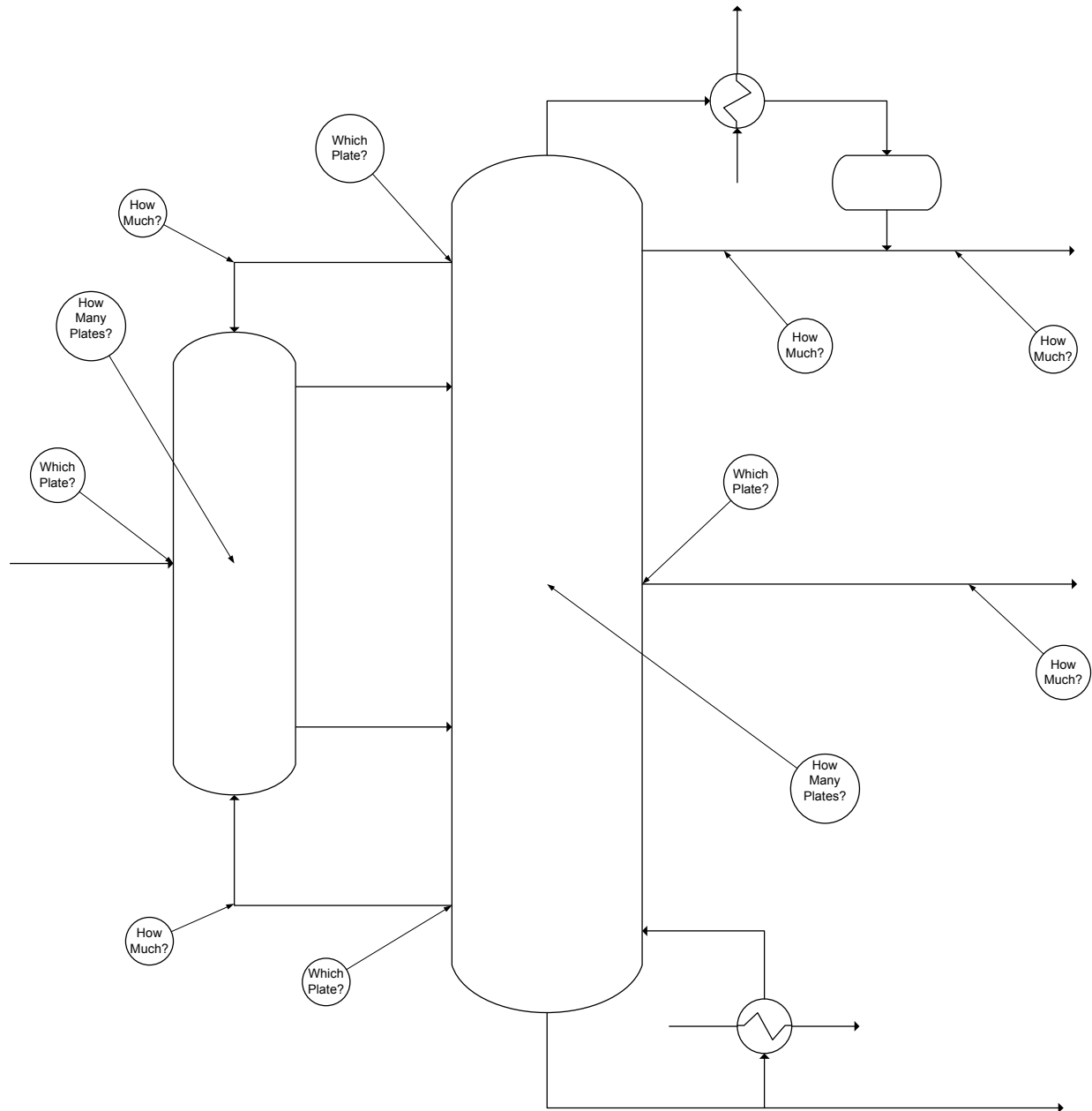
Figure 2.8 Key considerations when simulating a fully thermally coupled column.

The initial short-cut method of simulating a diving wall column as displayed by Triantafyllou and Smith (1992) would involve starting with three columns as suggested by the Direct sequence. The calculation carried out utilises the Fenske-Underwood-Gilliland short-cut techniques for multi-component mixtures with sharp separations. Some of the steps that then need to be followed are : Linking the column sections, Adjusting the number of plates in the pre-fractionator so that there are an equal number of stages in the prefractionator section and the side-draw section. Selecting the recoveries of the light and heavy key components in the pre-fractionator,

minimising the vapour flow for a given reflux ratio, then minimising the number of stages at a given reflux ratio and optimisation of the reflux ratio. The work by Triantafyllou and Smith (1992) also shows us that the results that they produce with the short-cut model is similar to those produced using a rigorous simulation engine. The short-cut method is thus suggested as an initialisation to rigorous simulation.

Once results of the short-cut method are available, the rigorous simulation can proceed by initially assuming that the total number of stages in the Petlyuk column is equal to the number of stages in the direct sequence. The next assumption would be that the number of stages on the feed and side-draw sides of the column are equal to half the total number of stages and that the locations of these streams are in the middle of the divided section. The total flow is then calculated based on the recovery and purity specifications on the products of the column. The variables that are usually manipulated are the reflux ratio and the internal reflux that controls the liquid flow to either side of the wall. The flow of the vapour however is dependant on pressure drop, on either side of the wall. If the same type of internals is used on either side of the wall then the vapour flow would be dependant on the areas on either side of the dividing wall.

The reflux ratio can then be minimised by adjusting the position of the feed and side-draw streams as well as the position of the dividing wall. In most cases it is preferable to specify an equal number of stages on either side of the wall in order to reduce the complexity of the problem and mechanical design as indicated by Linde AG (1998).

Results from repetition of this procedure using different total number of stages can be fitted using the Gilliland and Molokanov correlation from Wauquier (2000) developed to correlate reflux ratio vs. total number of stages.

$$Y = \frac{N - N_{min}}{N + 1} = 1 - \exp\left[\left(\frac{1 + 54.4X}{11 + 117.2X}\right)\left(\frac{X - 1}{\sqrt{X}}\right)\right]$$

$$X = \frac{R - R_{min}}{R + 1}$$

2.1

The parameters R_{min} and N_{min} are adjusted in order to fit the data and make it possible to calculate the optimum number of stages and reflux ratio using rules of thumb like equation 2.2 or equation 2.3.

$$N_{opt} = 2N_{min}$$

2.2

$$R_{opt} = CR_{min}$$

where C in equation 2.3 can vary between 1.1 and 1.5.

In order to minimise the energy consumption of the column, it is also desirable to minimise the vapour flowrate through the column. This can be done using the Underwood equations described in Wauquier (2000).

The short cut methods that have been outlined are then extended and refined in order to increase the accuracy of the design. The more rigorous models that have been developed require a lot of iterative computations to be carried out because of the many degrees of freedom in the design and operation of the column. Various methods have been proposed in order to curb the huge computational load and some of these methods will be outlined below.

The main reason for operational difficulty with a dividing wall column is the extra degrees of freedom that are present. It is often difficult to pair the appropriate manipulated and controlled variables. The dividing wall column has at steady state five degrees of freedom. The following may be selected as input manipulated variables: Boilup, reflux, side stream flow, liquid split to either side of the dividing wall and vapour split to either side of the dividing wall. There are only three main purity specification which are the top product, bottom product and middle distillate which leaves two extra degrees of freedom which can be used for optimisation purposes.

Design is also often done using commercial design packages like Aspen Plus™ or Hysis Process™ that carry out rigorous calculations in order to find the appropriate product specifications. These packages do not take into account the structure of the column in order to optimise the constructional and operational costs.

The methods outlined by Kim (2002) involve the structural part of the design being analysed using a rigorous tray by tray model before a steady-state simulation can be carried out. The structural information assists in eliminating the iterative computation that one encounters when using traditional design methods and software. Use of the optimum structure ensures that the best thermodynamic efficiency is achieved. When applying the method of structural analysis to a Petlyuk column, the factors that are taken into account are total number of trays and the locations of the interlinking and feed streams. The locations of interlinking between main column and any satellite column are determined by comparing the profiles of the liquid

composition in both columns. It is usually difficult to get an exact match between them, but the closest match is used to determine the location.

The degree of freedom analysis together with the tray by tray model allows for basic operability issues to be confronted before further design simulations are carried out. Once steady state simulations have been finalised dynamic simulations are undertaken to assess the operability of the column.

3. MODELLING OF DIVIDING WALL COLUMNS

3.1 INTRODUCTION

A model is a goal driven simplification of the reality obtained by abstraction as described by Halvorsen and Skogestad (1997). A process model is a model of a process, and its goal is to enable the simulation, analysis and understanding of a given process. This understanding is the prerequisite for improving already developed processes and for designing new, high quality processes.

Each of these processes taking place in a particular plant may be modelled in different ways which differ in the amount of detail included as well as the way in which the phenomena was interpreted. The freedom that exists contributes tremendously to the complexity of modelling undertaken. The specification of the model is related to the degree of understanding that the engineer may have of the process. Many software tools have been developed in order to assist the engineer in developing models of processes as well as increase the efficiency of the modelled process.

Typically a final process model is a collection of differential, integral and algebraic equations as well as mixtures of these types of equations. Depending on the degree of the detail included in the model and the complexity of the process being modelled, there can exist thousands of equations describing the system.

Simulation packages have generic building blocks that are commonly used, and in joining these blocks the engineer can build the model by connecting the appropriate blocks and streams together with correct property specification. The individual blocks have specified interfaces that allow for connections to be made. In certain cases where it is not feasible to use the generic building blocks, modifications may be made to these blocks in order to suit the process being simulated.

There are at present two methods that may be used in order to model a system. They are the use of equation-oriented software or block-oriented software. Equation oriented software is usually in the form of a declarative programming language, with some of them having a model library or a set of subroutine templates whereas block oriented software is based on a

flowsheeting level. The latter can be a bit restrictive because of restrictions that may be placed on the type of modifications that can be made to the standard models in the model library.

3.2   MODELLING OF A DIVIDING WALL COLUMN

Carrying out multicomponent distillation calculations is a tedious task because of the complexity involved.   There are, however, methods that can help the engineer to carry out these calculations in a rapid manner. Plate to plate and short-cut distillation calculations that include the use of absorption and stripping factors have been found to be reasonably accurate.

3.2.1   ABSORPTION AND STRIPPING FACTORS

The application of absorption and stripping factors has been well defined by Edminster (1957). The factors that affect the component distribution in multicomponent distillation are interstage vapour and liquid flows, K values and the number of theoretical stages.   These factors are generally derived by solving a mass balance and equilibrium balance to form absorption and stripping factors as follows:

$$A = \frac{L}{KV}$$ **3.1**

$$S = \frac{KV}{L}$$ **3.2**

Where   A   -   Absorption Factor

S   -   Stripping Factor

L   -   Liquid Flow

V   -   Vapour Flow

K   -   Equilibrium Constant

Functions of these factors, as well as number of stages, may be used in order to compute the component distributions. The absorption and stripping factors are generally constant in each of the column sections. These calculations may be carried out by using a plate to plate analysis, or by the use of effectiveness factors depending on the level of complexity needed. The method is considered to be rigorous if correct values of A and S are used for each stage in the calculations but for convenience mean values for A and S are used.

Each multi stage zone contains two feeds, the liquid coming from the top and the vapour coming from the bottom, as well as two products, the liquid leaving at the bottom and the vapour leaving at the top. The phenomena taking place in that section can be considered as absorption and stripping, where the liquid feed is subject to stripping from the rising vapour and the vapour feed is being absorbed by the liquid flowing down the column.

The method has can be simplified in order to undertake the calculations manually but is often solved using digital computer methods.

3.2.2   TRAY BY TRAY MODELS

The use of tray by tray models involves conducting material balances over each stage sequentially in order to model the column.   A general tray model that can be used will be outlined below:
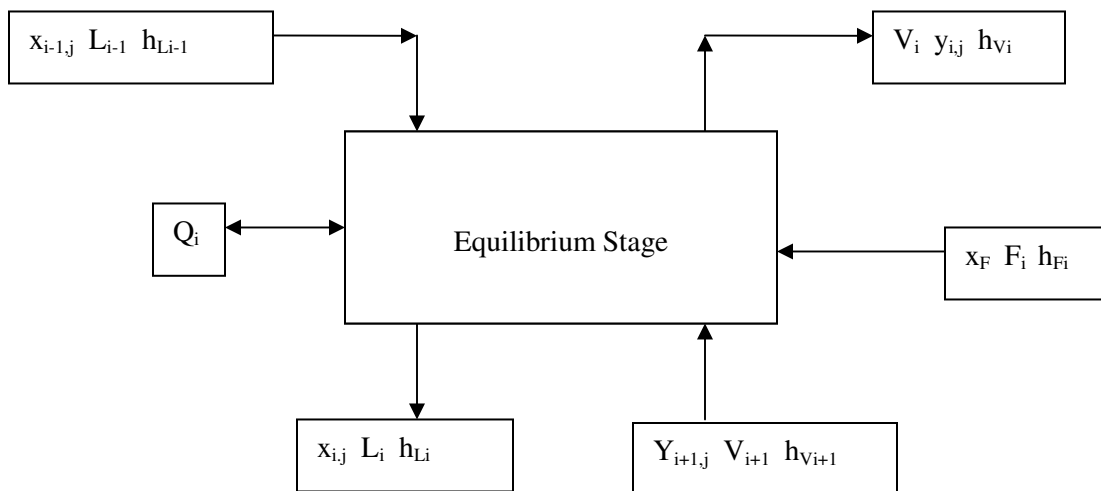
Figure 3.1 Generic model of a single tray, Treybal (1981)

Overall Mass Balance over Tray:

$$\frac{dM_i}{dt} = L_{i-1} + F_i + V_{i+1} - V_i - L_i$$

3.3

Overall Component Balance over Tray:

$$M_i \frac{dx_i}{dt} = x_{i-1,j}L_{i-1} + x_{F,j}F_i + y_{i+1,j}V_{i+1} - y_{i,j}V_i - x_{i,j}L_i \qquad \textbf{3.4}$$

Equilibrium Relationship on Tray:

$$y_{i,j} = K_{i,j}x_{i,j} \qquad \textbf{3.5}$$

Summation of Liquid Compositions:

$$\sum_j x_{i,j} - 1 = 0 \qquad \textbf{3.6}$$

Summation of Vapour Compositions:

$$\sum_j y_{i,j} - 1 = 0 \qquad \textbf{3.7}$$

Overall Heat Balance over Tray:

$$M_i \frac{dH_i}{dt} = L_{i-1}h_{Li-1} + V_{i+1}h_{Vi+1} + F_i h_{Fi} - L_i h_{Li} - V_i h_{Vi} - Q_i \qquad \textbf{3.8}$$

Where:

M_i	-	Overall Mass of components in tray i, (vapour and liquid)
L_i	-	Liquid Flowrate on tray i.
F_i	-	Feed Flowrate on tray i.
V_i	-	Vapour Flowrate on tray i.
$x_{i,j}$	-	Liquid Mole Fraction of component j on tray i
$y_{i,j}$	-	Vapour Mole Fraction of component j on tray i
K_i	-	Equilibrium Constant
H_i	-	Total Enthalpy on tray i
$h_{V/L,i}$	-	Vapour/Liquid Enthalpy on tray i
Q_i	-	Heat addition/removal on tray i

3.2.3 SIMULATION

A process simulation program usually improves the quality, speed and cost of designing processes. These tools hugely simplify the work of an engineer due to the fact that most complex computations have already been programmed into the software, which greatly reduces the time needed to generate a model. However, they are only as reliable and accurate as the level of complexity used to develop the model.

There are many steps involved in developing an appropriate model when modelling a system using simulation software. Initially a conceptual model is built ensuring that the basic equipment requirements are met, and then based on this a steady state model of the plant is built wherein validation and optimisation of the model is carried out to ensure that the actual plant conditions are being met. Once these have been carried out, dynamic modelling may be carried out in order to determine appropriate operability challenges as well as control strategies for the equipment.

Software available for simulation of chemical processes usually contains pre-defined models in a model library which need to be adapted in order to suit the needs of the particular process that needs to be simulated. Most simulation tools do not have models for dividing wall distillation columns in their model library, which means that the column needs to be decomposed into a form that would enable one to use the particular software. Of the many ways in which a dividing wall column may be decomposed, the two most widely used are displayed figure 3.2

The configuration depicted in figure 3.2 (a) is the configuration that was used in the Aspen Plus and Aspen Dynamic simulations created for the 1-Octene column. This configuration was chosen because it best suites the manner in which the simulation engine solves. The number of column sections used in the Aspen environment should be minimised because each individual column section used requires a sump to be specified. The streams joining the column sections require a driving force to move from one section to the other. The pressure profile of the column thus needs to be manipulated in each column section should one attempt to use the configuration in figure 3.2 (b) in an Aspen simulation.

Figure 3.2 (b) is was more suited to the modelling style used in the first principles model developed.
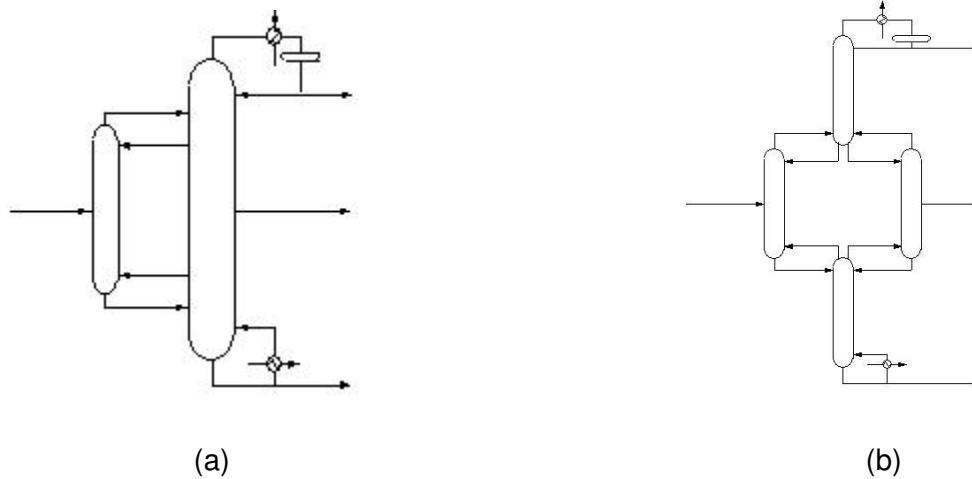
Figure 3.2   (a) The Petlyuk Configuration
                       (b) The compartment model

3.2.3.1 STEADY STATE SHORT-CUT MODELLING

In the initial stages of a project it is quite common to only have a limited amount of details pertaining to the plant that needs to be modelled. In order to overcome this problem one may use short-cut models to simulate the plant in question adequately. Short cut models can be relatively accurate depending on the operating conditions that are being simulated.

During these initial stages of the project these simulations provide valuable insight into the process as well as it gives the engineer a better understanding. Proprietary software such as Aspen Technology's Aspen Plus® may be used for this application.

There are two column types in Aspen Plus® that may be used in order to simulate using the short-cut methods. They are the DSTWU and the Distl where the former uses the Winn-Underwood-Gilliland method of solution, where one needs to specify the recovery of light and heavy key components, the number of theoretical stages and the reflux ratio. It then calculates the minimum reflux ratio, minimum number of theoretical stages, required reflux ratio and required number of theoretical stages. It also has the capability of estimating the optimum feed location as well as reboiler and condenser duties. The Distl on the other hand conducts its calculations based on the Edminster (1946) approach and assumes constant molar overflow and constant relative volatilities.

The software however does not cater of dividing wall columns which leads to one constructing columns like those in figure 3.2. These decompositions of the dividing wall column are accurate representations, provided that the heat transfer across the wall is negligible.

3.2.3.2 RIGOROUS STEADY STATE MODELLING

Traditionally it was preferred to use a short-cut solution method in order to obtain initial design estimates. The main reason for the use of these methods is that they are a lot simpler than rigorous design calculations, a lot quicker to apply and in most cases they provide a very good estimate from which to work. Yet as engineering has evolved into computer intensive environment it is now possible to perform a range of complex computations at the touch of a button.

Most packages these days offer the option of carrying out a detailed simulation. The model libraries contained in most process simulation packages contain a range of units, with different levels of detail present. At the moment most common pieces of equipment found in a chemical processing plant or refinery can be found in the model libraries of just about all simulation software with more specialised equipment being continually added to these packages. When one utilises Aspen Plus in the Aspen Engineering Suite the unit that one may use to perform detailed simulation of a distillation column is the Radfrac.

This model is highly specific, with built-in functionality that allows one to carry out all of the relevant detailed column calculations. It is also possible for one to include inter-stage reboilers and condensers for heat transfer as well as configure side strippers and rectifiers should the need arise. Peripheral equipment such as reboilers and condensers which are usually found in distillation systems may also be specified in detail. Another advantage of using this unit is that you control the amount of detail that you require. Basic information may be added to initially simulate the column and as more intricate information like tray type, efficiencies, sizes, packing ratings become available then they may be added to the simulation in order to increase the accuracy of the calculation.

The solution method used by Aspentech in the Aspen Plus package to solve the Radfrac is called the inside-out algorithm. This is described in detail in the Aspen Plus reference manual, Aspentech (2001). It consists of two nested loops. The K-value and enthalpy models specified

are only evaluated in the outside loop to determine parameters of simplified local models. The local model parameters are the outside loop iteration variables. The outside loop is converged when the changes of he outside loop iteration variables are sufficiently small from one iteration to the next.

The inside loop consists of the basic equations describing component mass balances, total mass balance, enthalpy balance, and phase equilibrium. These equations are solved to obtain updated temperature and composition profiles. The Radfrac unit adjusts the inside loop convergence tolerance with each outside loop iteration. The tolerance becomes tighter as the outside loop converges. The convergence methods used for this block are Bounded Wegstein, Broyden quasi-Newton, Schubert quasi-Newton and Newton.

The models produced by some software packages are so accurate that one may use the results from the simulation directly in order to make modifications to existing plants as well as design new plants. As the packages get more specific and rigorous the work load of the process engineer gets considerably lighter which allows the engineers to utilise their time on other matters as well.

3.2.3.3 DYNAMIC MODELLING

All the modelling concepts that have been discussed previously involve calculations based on a specific steady state of a process. The domain of dynamic modelling, however, operates quite differently. The aim of dynamic simulation is to predict the way in which the plant moves from one state to another. Predicting the transient response of a process is important when one considers factors such as Operability and Control.

Dynamic simulations are now used to predict the way in which a process and its control system would react to a disturbance. This allows the engineer the opportunity to analyse different control configurations on a particular plant such that the optimal configuration may be identified and implemented. Another area in which dynamic simulations have become very useful is in the simulation of plant start-up and shutdown sequences in order to identify critical areas where added attention would need to be focused upon.

Engineers are placing a lot of confidence in the accuracy of dynamic simulations because they are now based on fundamental engineering principles rather than transfer functions and contain detailed equipment models, rigorous thermodynamic data, actual hydraulic information for trays

and pipes, differential mass and energy balances as well as comprehensive controller algorithms. The controllers that are added to the simulation may be tuned and interaction between loops as well as control system stability may be assessed.

Another feature that makes these packages particularly attractive is the functionality that allows one to input custom models into the simulation, which is required in cases where new technologies are being analysed or when different vendor PID algorithms are being tested.

The value that can be gained from these simulations is immense, because critical design decisions may now be based on dynamic simulations which was not possible previously. The ability to analyse critical conditions like reactor effluent temperature in cases of runaway reaction, allows the design engineer the freedom to be less conservative.

Processes that are operating sub-optimally may be simulated in order to test the possibility of implementing advanced process control on these plants. In certain cases the actual advanced control package from the vendor may be connected to the simulation and the entire exercise of implementing a model predictive controller may be undertaken using the simulation. The models that are produced based on step tests undertaken on the simulation are in most cases so accurate that they may be used as initial models when step testing and developing models for the actual plant.

An important point to note when undertaking dynamic simulation of an existing facility is to ensure that the dynamic simulation is capable of being validated with the steady state model of the plant. This would help ensure that the results being used in order to make important design decisions are accurate.

4. CONTROL OF A DIVIDING WALL COLUMN

4.1   INTRODUCTION

The great need for separation in the chemical industry is the reason for such a vast number of distillation columns being in operation in chemical factories. Many of these columns are however not operating very well due to inadequate control system design. The best way to ensure that this does not occur is to improve the quality of the control system design so that the correct system is implemented the first time rather than troubleshooting in order to find solutions at a later stage when equipment has already been sized and installed.

The primary objective that is considered when designing a control system is to ensure that the regulatory controls that are designed for the system are adequate in order to maintain stable operation of the system. Traditionally the ideas governing control system design included trying to get the fastest response to set point changes and to try to compensate for disturbances as quickly as possible with a reasonable degree of loop stability. These days however the culture of control system practitioners is quite different with great importance being placed on designing a system that would have a dynamic balance between loops and minimum interaction rather than maximum speed of response.

Once this objective has been achieved and all the loops are operating well then one may choose to look for ways in which to optimise operation in order to maximise the workload on your asset and yield maximum profit from the unit. In some cases one may find that it is possible to run the unit at extremely high efficiencies with the basic regulatory layer of control whereas in other cases an advanced control system may be required. It is in these cases that advanced control methods may be considered.

4.2   INTEGRATED APPROACH TO COLUMN CONTROL

The approach taken when considering the 1-Octene distillation column was to design an integrated control system for the column. It involves many steps that will eventually lead to the development of a superior and more detailed control system design. Initially a steady state technique is used in order to screen the control possibilities. The method generally used is the

one proposed by McCune and Tolliver (1978), based on the Relative Gain Array by Bristol (1966). There are other differences in the methodologies that are utilised like ensuring that all the model specifications are mass flows rather than molar flows. Another convention is to stick to a philosophy of single point composition control rather than controlling the compositions on all product streams from the column. It is also expensive to measure the compositions of all streams exiting the column. The control strategy for the column is thus based on the most important component that needs to be recovered. The optimisation of all other variables on the column are done taking cognisance of the overall strategy. The benefits of increasing the complexity of control to more than single point control are not significant enough to warrant such a course.

4.2.1 DEVELOPING THE DESIGN BASIS

Before considering any control philosophies the control engineer needs to identify the specifications of the column and intent for which it was built.

The key factors that need to be identified are:
- The product composition specifications
- The constraints that need to be obeyed in order to meet specification
- The critical stream that is required to feed downstream operations
- The expected disturbances to the column
- Operation Constraints
- Identifying the conditions and constraints for normal operation of the column.

These factors form the core strategy for column control, which the philosophy for designing the control system is based on.

4.2.2 SELECTING CANDIDATE CONTROL SCHEMES

The first step that is involved in selecting a control scheme involves identifying the degrees of freedom in the system. These degrees of freedom represent the manipulated variables in the system. Once this is done one proceeds to distinguishing the demand streams in the system, i.e. those streams whose rate is set by other operations either upstream or downstream, or the stream that is required to achieve a certain composition specification. The relative size of the bottoms stream and boil-up streams are taken into account when selecting which should be used to control the level in the sump.

When considering the alternatives one should keep in mind what effects the individual loops in the chosen scheme would have on each other. Attempts should be made to try to eliminate or minimise the amount of interaction present in the column.

The overall control philosophy that was designed by Linde AG for the 1-Octene column was intended to produce a C_8 side draw meeting the required 1-Octene purity and recovery as inferred from temperature measurements.

The quantity of reflux to the column is controlled by a temperature differential controller measuring the temperature difference between the section of the column above the partition and the overhead vapour system cascaded onto a flow controller. As the temperature differential increases the quality of reflux is increased. The distillate is removed on level control from the reflux drum.

A temperature differential controller was used in preference to a temperature controller because the air cooled condenser can cause sudden pressure variations when ambient conditions change suddenly as is the case for a thunderstorm.

The flow of the main product in the vapour side draw was on flow control whereby the set point is corrected by the temperature difference between the overhead vapour and the liquid temperature in the partitioned section below the vapour draw.

The bottom product from the column is a C_9 stream that is removed via level control. The heat from the bottoms product in the column is used to heat up the feed to the column in a feed product heat exchanger.

The column pressure is controlled by a split range controller. Primarily the pressure is controlled by varying the degree of flooding in the tubes of the condenser. When this is insufficient the inert components in the reflux drum are vented to the flare system. For situations of low pressure a nitrogen injection system is installed in the condenser inlet stream. A hot vapour bypass is also used to stabilise pressure in the reflux drum.

4.2.3   TESTING THE SELECTED CONTROL SCHEMES

The open loop testing procedure is run in order to determine the sensitivity of the key components to temperature so that temperature may be used as a controlled variable in order to infer product purity.

It is during this phase that dynamic simulation would be considered in order to identify the appropriate control points. It would not be possible to undertake such analysis once the actual column has been constructed because control systems are installed during the construction phase and not after commissioning the column.

In most cases it is also common practice to place additional temperature measurements one theoretical stage above and below the specified temperature measurement. This is to ensure that any slight uncertainty in the modelling would be taken into account as well.

After identifying the key control points, hold-ups and other key dynamic information may be added to the model in order to test the sensitivity of the candidate control scheme in closed loop. Typical disturbances that the process is expected to experience are simulated in order to determine whether the scheme is capable of handing it. Some of the other candidate control schemes are also tested subject to the same disturbances and the performance of these schemes may be compared.

4.3   CONTROLLABILITY OF COMPLEX COLUMNS

Most of the research carried out on these columns has been directed towards designing energy efficient systems with little effort being directed towards operability and controllability. Extensive research has shown that these columns are highly attractive with respect to conservation of energy. The next step is to show whether or not these columns are still as attractive after operability and control have been researched.

Control studies on more complex distillation configurations began by analysing the systems in order to determine the amount of interaction present. The preliminary studies undertaken by Ding and Luyben (1990) have shown that even though a certain degree of coupling is present, the columns are still controllable. The study included a prefractionator setup as well as a Petlyuk column setup as indicated in figures 2.5 and 2.6 respectively. The control structure was limited to a Single-input-single-output (SISO) multiloop structure. Non-linear and multivariable controllers were not included in the study.

The process of determining whether or not the system is controllable begins by analysing the system and conducting a Degree of Freedom (DOF) Analysis. The degree of freedom analysis is done in order to determine number of control loops required in order to control the column.

The degrees of freedom analysis undertaken by Abdul Mutalib & Smith (1998), reveals that a dividing wall column has two extra degrees of freedom as compared to a conventional distillation column. The two additional manipulated variables would be vapour and liquid split above and below the dividing wall. The vapour split cannot be directly manipulated during operation of the column because one would be required to shift the position of the dividing wall in order to effect changes.

During normal operation the vapour split inside the column occurs naturally according to the pressure drop relation across the internals on either side of the wall. This means that if there are an equal number of stages on either side of the column then the vapour split would be governed by the position of the wall and the liquid loading on either side of the wall.

The distribution of internal liquid reflux between the feed and product sides of the column is a powerful design and control variable. There is an optimal distribution that needs to be maintained for each separation task. In practise the vapour distribution is generally symmetric while the liquid distribution is asymmetric.

To bring about the desired column performance with the optimal flowrate of reflux on each side of the partition it is essential that the vapour distribution occur as intended by the designer. This requires the internals to be specified, manufactured and installed in such a way that the pressure drop on either side of the partition can be equal for the desired vapour distribution as described by Bekker (2001).

The liquid split can be effectively manipulated to control the column. This is done by carefully calculating the position of the dividing wall. The area ratio between either side of the column should be equal to the vapour split required to optimally operate the column.

The optimum conditions for operation of this type of column should be carefully calculated during the design stage. The column should then be operated very close to these conditions. Simulations have shown that varying the liquid spilt of the column could end up becoming a costly exercise due to energy costs in the reboiler associated with the extra liquid loading.

Dividing wall columns have two liquid reflux points on the column, one being from the chimney tray just above the partition and the other a conventional column reflux at the top of the column.

The two control strategies that are most commonly used is either direct composition control using analysers to measure product compositions or temperature control which works on the principle of inferring the product compositions. Temperature control is not always possible especially in cases where there are negligible temperature gradients across the column. The method most commonly used to find the ideal temperature measurement locations is the temperature profile analysis. Fixed changes are made to the manipulated variables and the corresponding changes in the temperature profile of the column are analysed. Singular value decomposition may also be used to find or confirm the optimum location for the temperature measurements.
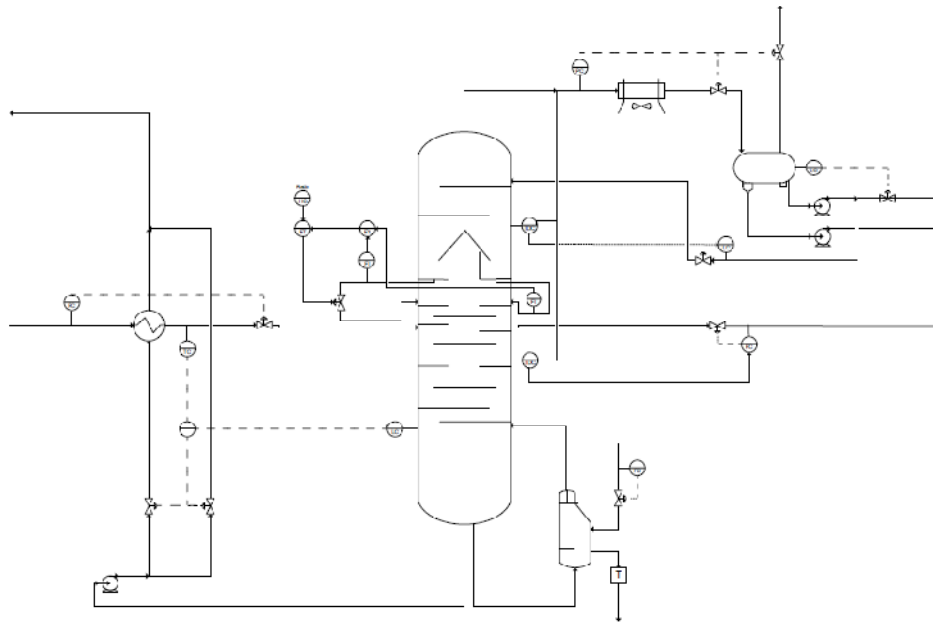
Figure 4.1 P&ID of the basic control system for the 1-Octene column

The basis for the basic control system strategy is to maximise the recovery of 1-octene in the sidestream taken from the column. The secondary driver is optimisation of utilities used in the production of this product. The 1-octene prefractionator column is the first in a train of multiple distillation columns that are used to purify the final 1-octene product.

The pressure control on the column is designed to maintain a constant pressure during operation. The system is referred to as a "Nitrogen push – pull" system. The split-range control

strategy releases vapour from the overhead separator to a flare system in instances of overpressure and inject Nitrogen into the overhead vapour stream to increase pressure in the overhead system. The column is designed at a pressure of 4 bar to ensure that vented products can be discharged into the factory flare system which is designed for 4 bar. Relief of vapours from the system is also discharged to the flare system in cases if emergency,

The flow to the column is controlled via a flow controller that is set by the operator and the temperature of the feed is maintained by a hot bypass in the feed product heat exchanger. The heat load delivered to the column is set by the operator by manipulating the flow of steam to the reboiler. The inventory in the sump is controlled using a level controller cascaded to the feed temperature controller. The level controller manages the total product flow out of the column while the temperature controller decides on the relative amount that bypasses the exchanger in order to maintain feed temperature.

Internal reflux to either side of the wall is maintained at a ratio that is predetermined during design for optimal separation. The absolute flow to the product side of the column is set by the operator to ensure sufficient liquid loading on the trays such that the trays do not run dry. The flow to the other side automatically corrects itself and maintains the pressure balance on either side of the wall.

The dual differential temperature measurements are both aimed at recovering the maximum amount of 1-octene. The upper differential temperature is calibrated to increase the flow of sub-cooled reflux when 1-octene moves up the column above the side draw. The lower differential temperature measurement is cascaded to the flow of 1-octene out of the column. The flow out of the column is throttled when heavier products move up the column as detected by an increase in differential temperature.

The relative gain array method has been used to determine the amount of interaction present in the system. Irrespective of the type of control arrangement one chooses for this type of column, a certain amount of interaction would be present. If one chooses to attempt controlling a dividing wall column with only PID controllers then one would need to tune the controllers in order to negate the effect of interaction.

Processes with complex dynamics and interaction are perfect candidates for Advanced control. The use of advanced control for dividing wall columns will avoid the problems of interaction expected in multiple-loop control.

5. ADVANCED CONTROL

5.1   INTRODUCTION

Over the past thirty years much has been written about advanced control; it's underlying theories, the practical application and the projection of future trends.   During the 1960's advanced control was taken to mean any algorithm or strategy that deviated from classical PID controller.   Nowadays advanced control is synonymous with the implementation of computer based technologies.

Measurement is the gathering of information from the process that will guide the decision of what to control.   Control is the manipulation of the process degrees of freedom in order to satisfy the operation criteria.   Optimisation is a technique of manipulating the process degrees of freedom to satisfy the plant economic objectives.   The same set of variables are manipulated in order to control and optimise the process.

Depending on an individual's background, advanced control may mean different things. It could be the implementation of cascade control schemes, adaptive algorithms, optimisation strategies or one of many other control techniques.

With most processes there are many variables that need to be regulated. Multivariable control should be considered for systems where interactions occur.   Of the multivariable control technologies available Model Predictive Control (MPC) is the most widely implemented advanced control technology.

MPC refers to a class of computer control schemes for the explicit prediction of future plant behaviour. Process inputs are computed so as to optimise future plant behaviour over a time interval known as the prediction horizon.

In recent years the MPC landscape has changed drastically with a striking increase in the number of applications. Control algorithms are highlighted in this section of the thesis.

5.2   MODEL PREDICTIVE CONTROL (MPC)

The essence of MPC is to optimise the forecasts of process behaviour using the identified controlled variables (CV's) and Disturbance Variable (DV's).   The forecasting is achieved with the use of a process model, which highlights that the model is a fundamental element of an MPC controller. As it will be seen later, models are not perfect forecasters and hence feedback is used in order to overcome some of the effects of poor models.

The strong position that MPC has achieved in most industrial fields is due to the design procedure and the ease with which this method handles the process model. Another strong motivating factor for MPC is that constraints on variables may be handled at the design stage. Most companies offering MPC solutions have also gone a long way to make these software packages easy to use.

One of the main principles on which MPC is based is that the plant dynamics are described by an explicit process model, which can take any required mathematical form. Process input and output constraints are included directly in the problem formulation so that future constraint violations are anticipated and avoided.

At each control interval the algorithm attempts to optimise future plant behaviour by computing a sequence of the future set of manipulated variable adjustments. The first input in the optimal sequence is then sent to the plant and the entire calculation is repeated for future control intervals. In many industrial implementations the desired targets are calculated as a steady state economic optimisation at plant level. In these cases the desired targets are normally constant between plant optimisations which are performed on a slower time scale to the one at which the MPC controller operates. Thus the MPC is able to track the targets set by the plant optimiser.

The general objectives of an MPC controller are to prevent the violation of input and output constraints; drive the CV's to their steady-state optimal values; drive the MV's to their steady-state optimal values using the remaining degrees of freedom; prevent excessive movement of the MV's and when signals and actuators fail, to control as much of the plant as possible.

The translation of these objectives into a mathematical problem involves a number of approximations that define the basic character of the controller. Like any design problem there

are many possible solutions and hence a lot of different approaches have been taken in the field of MPC control. Some of the techniques researched are outlined below:

5.2.1   LQG (Linear Quadratic Gaussian)

The ideas and concepts outlined by R.E. Kalman(1960), in the early 1960's has revolutionised the field of control theory and has become pervasive in engineering systems. The Kalman filter is a recursive state estimation technique. It is capable of providing estimates of measured and unmeasured system state variables which is a compromise taking into account the expected errors in the measurements and the model. From incomplete information, it can optimally estimate and control the state of a changing, complex system over time. It is a recursive data processing algorithm from which optimal estimates are generated from a set of measurements.

The LQG/Loop Transfer Recovery (LTR) is an optimal control method that can be applied to linear time-invariant single input single output (SISO) and multiple input multiple output (MIMO) systems. This feedback control system has good robustness properties such as a reasonably large stability margin, good disturbance attenuation and a low sensitivity to parameter variations.

The LQG structure consists basically of a Kalman filter state estimator and a linear quadratic regulator (LQR) as shown in figure 5.1. The plant disturbances and measurement noise are represented by two uncorrelated white noise processes $w(k)$ and $v(k)$ respectively with normal (Gaussian) distribution and zero mean. The Kalman filter estimator, by design has been shown to have good robustness properties for plant perturbations at the plant output whereas the LQR has been shown to have good robustness properties for perturbations at the plant input. In spite of the fact that the individual components of the LQG has good robustness properties, the LQG controller collectively as a structure would not guarantee robustness properties at either the plant input or the plant output as described by Kwakernaak and Soderstrom (1983).
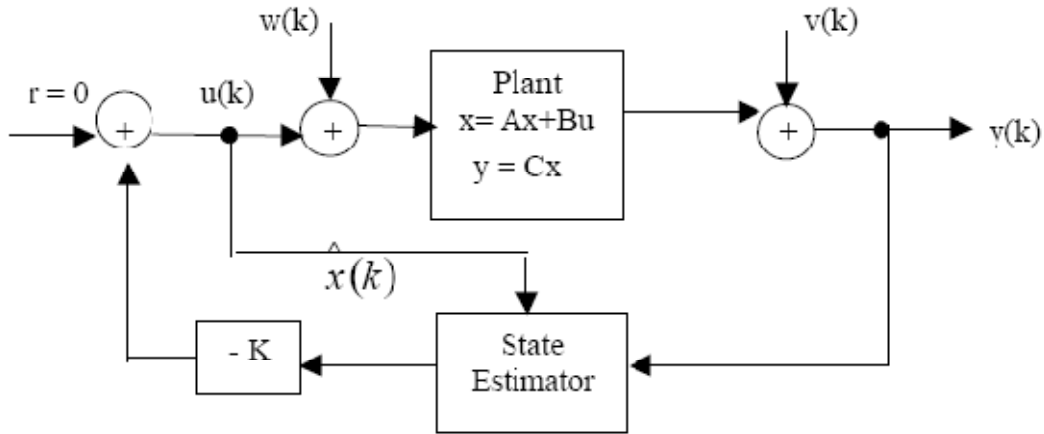
Figure 5.1 Simplified LQG block diagram by Vegte (1994)

In the linear quadratic regulator problem, the plant is represented by a linear state space model either as time-variant or as time-invariant, depending on the dynamic behaviour of the plant. Considering the case of discreet linear time-invariant form of the plant, the state space model is usually expressed by state difference equation and output (observation) equation as:

$$x_{k+1} = Ax_k + Bu_k \quad \text{where k = 0, 1, 2, 3 ....N} \qquad \textbf{5.1}$$

$$y_k = Cx_k \qquad \textbf{5.2}$$

The objective in designing an optimal control system is to determine control law u(t) that is optimal in some sense in order to obtain a desired plant performance. In the LQR algorithm, the control input to the plant takes the optimal form:

$$u_k = -Kx_k \qquad \textbf{5.3}$$

Where K is an optimal gain schedule that needs to be calculated based on minimising a quadratic cost function in the form:

$$J_N = \sum_{k=0}^{N} (x_k^T Q_k x_k + u_k^T R_k u_k) \qquad \textbf{5.4}$$

Where :

X_k The State Vector

U_k Vector of Control Inputs

Y_k Vector of Measurements

K Optimal Gain Schedule

Q_k Weighting matrix

R_k Weighting Matrix

J_N Quadratic Cost Function

Where N is finite and Q_k and R_k are positive definite and positive semi definite weighting matrices respectively. Both matrices are usually selected to be symmetric to simplify the computation without an loss of generality. These matrices define the trade-off between regulation performance and control effort. The quadratic cost function in equation 5.4 is considered for the simplicity in its development and computations as well as the logical sense it offers, through the flexibility in selecting Q and R to obtain the desired performance. Minimising the first term of equation 5.4 ensures that the states will be driven to the zero state as quickly as possible, whereas minimising the second term will ensure that the control u will not be too large for all practical purposes.

If the measurement seems to be reliable then the measurement co-variance decreases to zero. The residual is thus weighted more than the prediction. And if the prediction is seen to be more reliable then the prediction error co-variance decreases to zero and the prediction is weighted more heavily than the residual.

The LQG design when it is considered in conjunction with the LTR procedure serves to recover robustness at either the input or the output of the plant. If robustness is desired at the input of the plant, the first consideration is to design a nominal robust LQR satisfying the design constraints. Consequently, an LTR design procedure should be incorporated by designing a Kalman filter gain that recovers the robustness at the input to the plant to approximate that of the nominal LQR design. If, however, robustness is desired at the output of the plant, a nominal robust Kalman filter design is made to satisfy the performance constraints. Consequently, an

LTR design procedure is used to design an LQR gain that recovers robustness at the output of the plant to approximate that of the nominal Kalman filter design.

The Kalman filter gain is computed from the solution of a matrix Riccati equation. The controller gain can also be found by constructing a dual Riccati equation, so that the same numerical techniques and software may be used for both calculations. The infinite prediction horizon of the LQG algorithm endows the algorithm with powerful stabilizing properties. The main problems however involved with LQG theory are constraints handling, process nonlinearities, model uncertainty and unique performance criteria.

The economic operating point of most process units lies at the intersection of constraints. A successful controller should thus be capable of maintaining the system as close as possible to the constraints without violating them. A more general model-based control methodology would solve the dynamic optimisation problem online at each control execution. Process inputs are computed so as to optimise future plant behaviour over a time interval known as the *prediction horizon*. Process input and output constraints may be included directly into the problem formulation so that future constraint violations are anticipated and avoided. The first input of the optimal input sequence is injected into the plant and the problem is solved again at the next time interval using updated plant data. Empirical plant models may also be developed from test data and this may be used, substantially decreasing the cost of developing rigorous first principles models.

The LQG is a form of predictive control that does not address the problem of constraints. It is for this reason that other methods are investigated.

5.2.2   DYNAMIC MATRIX CONTROL (DMC)

Cutler and Ramaker (1979) presented details of an unconstrained multivariable control algorithm which they named Dynamic Matrix Control (DMC). The key features that the DMC algorithm presents are the linear step response model for the plant, quadratic performance objective function over a finite prediction horizon, future plant output behaviour specified by trying to follow the setpoint as closely as possible and optimal inputs computed as the solution to a least squares problem.

The linear step response model used by the DMC algorithm relates changes in a process output to a weighted sum of past input changes referred to as input moves. By using the step

response model one can write future output changes as a linear combination of past and future input moves. The matrix that ties the two together is the *Dynamic Matrix*. Using this representation allows the optimal move vector to be computed analytically as the solution to a least squares problem. Feedforward control is readily included in this formulation. In practise, the required matrix may be computed offline to save computation. Only the first row of the final controller gain matrix needs to be stored because only the first move needs to be computed.

The objective of a DMC controller is to drive the output as close to the setpoint as possible in a least squares sense with a penalty term on the MV moves. This results in smaller computed input moves and a less aggressive output response. This technique provides a degree of robustness to model error. Move suppression factors also provide an important numerical benefit in that they can be used to directly improve the conditioning of the numerical solution.

Certain developers of DMC technology also made use of time variant constraints whereby an extra equation is added to the process model when a predicted input comes close to an absolute constraint. This usually drives the input back into the feasible region and prevents violation of absolute input constraints but this requires changes to be made on-line so the dynamic matrix inverse solution needs to be done on every control execution.

To try and reduce computational complexity Prett and Gilette (1980) developed a tearing solution that allowed them to compute the original matrix inverse offline and only perform online computations when the time variant constraints are triggered.

5.2.3   QDMC

Cutler, Morshedi, and Haydel (1983) developed the QDMC algorithm, where the key distinguishing features were its linear step response model for the plant; quadratic performance objective over a finite prediction horizon, future plant output behavior specified by trying to follow the setpoint as closely as possible subject to a move suppression term and optimal inputs computed as the solution to a quadratic program. This enables the future projected outputs to be related directly back to the input move vector through the dynamic matrix. This allows all the input and output constraints to be collected into a matrix inequality involving the input move vector.

Even though the QDMC algorithm is quite a complex control algorithm, the QP itself is one of the simplest possible optimisation problems that one could propose. The Hessian of the QP is

positive definite for linear plants and so the resulting optimisation problem is convex. This means that the standard solution can be found readily using standard commercial optimisation codes or packages. The use of the second generation QDMC algorithm developed by Garcia and Morschedi (1986), also enables the controller to perform well when it comes to online optimisation. It provides a smooth transition from one constrained operating point to another.

The QDMC algorithm provides a systematic approach to incorporate hard input and output constraints but there is no feasible way to handle an infeasible region. The formulation of soft constraints meant that certain constraints could be violated to some extent as decided by the relative weights of the constraints.

5.2.4   FAULT TOLERANCE

Fault Tolerance is also an important practical issue when designing a controller. A practical MPC controller should not just go offline and relinquish control to the basic control system when signals are lost but it should rather remain online and try to make the best of the sub plant that it has under its control. A major problem that is encountered when attempting to achieve this is the fact that a well conditioned multivariable controller may have ill conditioned sub processes that run beneath the advanced process control layer. A proper control monitoring maintenance programme should be in place to recognise and screen out these problems before they result in bad control. When one analyses all the control requirements of a plant and the weights that need to be assigned to the value of output setpoint violations, output soft constraint violations, input moves and optimal input target violations, one will realise that it is not easy to translate control actions into a set of consistent weights. In some cases it would not make sense to include these in the same objective function because driving inputs to their optimal targets may lead to a larger violation of output soft constraints. Even in cases where a consistent set of weights are found for a controller, care should be taken to ensure that there are no scaling problems that could lead to an ill conditioned multivariable controller.

New advancements needed to be made to previous algorithms in order to attempt to address these new practical issues that were arising from industrial operations. The hallmark of the newer DMC algorithms are that they are equipped with the following tools as part of their service offerings:
- linear impulse response model of the plant
- Controllability supervisor to screen out ill conditioned plant subsets

- Multi-objective function formulation
- A quadratic output objective function followed by a quadratic input objective
- Constraints can be hard or soft, with hard constraints ranked in order of priority.

Physical systems are naturally represented using state-space model structure. Real processes have internal connections and can exhibit a range of fast and slow dynamics, including integrating and unstable modes, all of which are described in a state space structure. State estimation provides the mechanism to detect disturbances entering into the plant. In the implementation of MPC, process conditions sometimes arise where there is no solution to the optimisation problem that satisfies the constraints. Rather than declaring such situations process exceptions, it would be preferable to find a solution that enforces some of the inequality constraints while relaxing others to retain feasibility. It is quite common to find that these input constraints represent physical limitations like valve saturation that cannot be violated. Output constraints, however, generally do not represent hard physical boundaries but rather desired ranges of operation that can be violated when necessary. In order to avoid infeasibilities, output constraints are thus relaxed and treated as soft constraints.

A quadratic output objective function is minimized first subject to hard input constraints. Each output is driven as closely as possible to a certain value at a single point in time known as the *coincidence point*. The name comes from the fact that this is where the desired predicted values should coincide. The desired output value is predicted using a first order reference trajectory that starts at the current measured value and leads smoothly to the setpoint. Each output has two basic tuning parameters; a coincidence point and a closed loop response time used to define the reference trajectory.

Currently, performance from state estimation comes at a price of defining a disturbance model and tuning the resulting filter. State estimates are best done using directly measured outputs and not calculations. The core plant state-space model should simply relate measured outputs to measured inputs in order to describe the state equations most efficiently. An improved numerical solution engine would help solve the sequence of separate steady-state target optimisations and also incorporate multiple ranked control objectives. An explicit disturbance model describes the effect of unmeasured disturbances. A Kalman filter is used to estimate the plant states and unmeasured disturbances from the output measurement. A distinction is introduced between controlled variables appearing in the control objective and feedback

variables that are used for state estimation. This allows the input and output constraints to be enforced by a QP formulation.

The latest generation of DMC technology available commercially today has features such as:

- windows based graphical user interfaces
- multiple optimisation levels to address prioritised control objectives
- additional flexibility in the steady-state target optimisation, including QP and economic objectives
- direct consideration of model uncertainty and improved identification technology based on prediction error method and sub space identification methods
- Subspace algorithms that support State-space model identification.
- Infinite horizon controllers where the future trajectory is calculated by evolving the state estimate into the future.

5.2.5 CONTROLLER DESIGN AND TUNING

In order to design a controller the ideal starting point would be to define the size of the impending controller by determining the relevant CV's, MV's and DV's. This can be done in accordance with the stated control objectives of the plant. The next step would be to test the plant by systematically varying the MV's and DV's in order to capture and store the real-time data showing how the CV's respond. The dynamic model of the plant is then constructed either from first principles or using plant test data and an appropriate identification package. This is sufficient for one to enter initial tuning parameters into the controller to configure it, which would lead to testing of the controller in an offline closed loop simulation environment. Controller performance can thus be verified. The next step would be to download the final configured controller to the destination machine and test the model predictions in open loop mode. Finally, once one is happy with the installation, one may put the controller online and tune it where needed.

A lot of time is usually spent in the closed loop simulation step to test the verification of acceptable performance of the controller. The tests are generally performed to check the responses of each CV as well as the way in which the system would respond to violations of major constraints. The final tuning step then follows during which the controller is tested for robustness to model mismatch by varying the gains and dynamics of key process models.

However one should note that irrespective of how much of testing is carried out, it is usually impossible to simulate or test every possible scenario that may occur.

The need to have MPC control technology that is robust when it comes to various types of uncertainty and model error is of paramount importance. The difficulty in MPC usually occurs in the open loop nature of the optimal control problem and the implicit feedback produced by the receding horizon. There are adjustable parameters in MPC controllers that allow for tuning of the controller. The parameters are:

- Sample time
- Model Horizon
- Controlled variable weights
- Finite Prediction Horizon
- Control Horizon
- Move suppression co-efficeints

The tuning challenge presented by this array of adjustable parameters is significant since many of the parameters have overlapping effects on closed loop performance.

5.2.6   ACQUIRING MV, CV AND DV VALUES FROM THE PROCESS

The first action of any controller is to read the current state of the plant inputs (MV's and DV's) as well as plant outputs (CV's). Most newer plants are equipped with SMART instrumentation that is capable of transmitting multiple signals along the control network. In addition to the actual control signals sent to the DCS, other valuable information like sensor status to check fidelity of the reading is also sent. MV's usually carry information relating to the status of the valve together with its control signal. In the case of MV's being unreliable, like cases of valve saturation, then the MV will only be allowed to move in one direction only. When an MV is disabled and cannot be used for control purposes it can be considered by the rest of the advanced controller as a measured disturbance (DV).

5.2.7   OUTPUT FEEDBACK

In this step of the control execution the controller makes use of the available measurements in order to estimate the dynamic state of the system. The best way in which to handle this issue

would be to utilise Kalman Filter concepts but industrial MPC controller developers have rather chosen to use a different approach that involves comparing the current measured output to the current predicted output which gives rise to a bias term that is used in most algorithms.

The Kalman filter requires all the system characteristics such as system model, initial conditions and noise characteristics be specified a priori. Due to the fact that uncertainties in these variables do exist in real processes the kalman filter is not preferred as described by S. Sasa (1998).

The use of the bias term gives rise to new problems like the need for input and output disturbance models to counteract the problem of not having feedback for the process state estimates and identity feedback for the output disturbance. Industrial controllers have thus chosen to take the route of using ad-hoc fixes in order to deal with issues that arise like in cases when the CV measurement is not available. A typical solution would be to skip the bias update for a certain number of control intervals and if it remains a problem over a period of time then control of the CV is disabled.

5.2.8 DETERMINING THE CONTROLLED SUB-PROCESS

The controller must decide which MV's can be manipulated and which CV's can be controlled once the process dynamic state has been estimated. In cases where the CV status is bad or if the operator has disabled the control of a particular variable then it may be excluded from the control execution. Hard constraints may be imposed on MV's if the lower level function of the MV is inhibited like in the case of a saturated valve but when MV's are found to be disabled then they are treated as DV's. The controlled sub- processes change in real time which illustrates the importance of allowing extra degrees of freedom in the controller design.

The route followed by most developers is to prioritise the faults that occur during control. The entire controller would only shed (relinquish control back to the basic DCS control system) in practise when a critical CV fails.

5.2.9 REMOVAL OF ILL-CONDITIONING

In the application of DMC to a large scale process, a large number of dynamic process models are prepared through several identification tests in order to construct the internal models used for output prediction. Some models show a small steady-state gain. Of these models several may be deemed as negligible for designing the internal models of the predictive controller. It is

difficult to determine at the designing stage whether the future control performance of the plant will deteriorate by neglecting the small gain models. Whether or not to include the models into the final controller design is decided based on operational knowledge and experience on the plant.

Neglecting one model sometimes causes the excessive input movement at some particular control execution and may end up causing an unstable control system. Conditioning of the entire controller is usually checked when designing the controller but it is almost impossible to check all the possible sub-processes. In any particular control execution there may exist a scenario where the controller would require huge input movements in order to control the outputs independently. It is therefore important to examine the condition of the sub processes at each control execution to remove ill conditioning.

Initially the DMC LP controller was developed to deal with this problem. It used linear programming to perform the local steady state optimisation subject to hard input and soft output constraints. The manner in which it operates is can be described as selecting an equal number of controlled and manipulated variables from the full scale non-square process, and controlling the selected square process.

Two other methods used to accomplish this are single value thresholding or input move suppression.

5.2.10 LOCAL STEADY STATE OPTIMISATION

The DMC algorithm can be separated into two parts, a predictor and an optimiser. By splitting up the algorithm in this manner, similarities with state-observer state feedback controllers become apparent. Unconstrained DMC is equivalent to an optimal state observer (Kalman Filter) and linear quadratic feedback, using a receding horison approach and special assumptions about disturbances and measurement noise.

The internal model of the DMC predictor, does not yield an estimate of the true plant output. It computes the open-loop model output, for previous input moves, but does not account for the effect of disturbances and model plant mismatch.

A separate local steady state optimisation is usually carried out at each control cycle to compute steady state input, state or output targets. This is necessary because optimal targets may

change at any time due to disturbances entering the process or operator inputs that re-define the control problem.

The optimisation problem is typically formulated to drive steady state inputs and outputs as closely as possible to targets determined by the local economic optimisation without violating input and output constraints.

5.2.11 DYNAMIC OPTIMISATION

An MPC controller must compute a set of MV adjustments that will drive the process to the desired steady state operating point without violating constraints. Most MPC developers choose to minimise the dynamic objective function subject to model constraints.

There are three types of constraints that occur in most industrial controllers.   These are hard, soft and setpoint approximation.   Hard constraints are those that should never be violated whereas soft constraints may be violated to some extent but they are generally minimised using a quadratic penalty in the objective function.   Setpoint approximation of a constraint involves penalising deviations above and below the constraint.   This has been described by T.F. Edgar (2004).

The objective function is usually in the form of a quadratic program that can be solved using commercially available software.

5.3   PROCESS MODELS

Model development is by far the most critical and time consuming step in implementing a model predictive controller.   Historically the models of choice in early MPC applications were time domain, input/output, step or impulse response models.   Models of this form were easy to understand for control engineers and hence they gained wide acceptance in the industry.

The technical scope of an MPC development is largely defined by the form of the process models that it uses.   Empirical process models are models that are usually constructed exclusively from test data and it is because of this that they generally cannot be expected to accurately predict process behavior beyond the range of the test data used to develop them. First principle models are derived from purely theoretical considerations such as mass and

energy balances and are typically much more expensive to develop. They do however allow you to predict plant behavior over a much wider range of process operation.

It is in most cases very difficult to get process models that are purely first principle models. In most cases first principle models are calibrated using process data to estimate key parameters and often empirical models are adjusted to account for known process physics. The actual form of the models may be broken up into different categories:

5.3.1 NONLINEAR FIRST-PRINCIPLES MODELS

The use of nonlinear models in MPC is motivated by the possibility or improving control by improving the quality of the forecasting. The fundamentals of any process control problem are defined by conservation of mass, momentum and energy, and consideration of phase equilibria, relationships of chemical kinetics and properties of final products. Each one of the factors mentioned above introduces a certain level of non-linearity into the system. Hence there is a need for nonlinear models to accurately describe these phenomena.

Optimisation over inputs subject to hard constraints leads immediately to nonlinear control, and the departure from well understood and well tested linear control theory.

These types of models are derived from mass and energy balances and take the forms shown below:

$$\overline{\dot{x}} = \overline{f}(\overline{x}, \overline{u}, \overline{v}, \overline{w}) \qquad\qquad \textbf{5.5}$$

$$\overline{y} = \overline{g}(\overline{x}, \overline{u}) + \overline{\xi} \qquad\qquad \textbf{5.6}$$

Where $u \in \Re^{m_u}$ is a vector of MV's, $y \in \Re^{m_y}$ is a vector of CV's, $x \in \Re^n$ is a vector of state variables, $v \in \Re^{m_v}$ is vector of measured DV's, $w \in \Re^{m_v}$ is a vector of unmeasured DV's like noise and $\xi \in \Re^{m_\xi}$ is vector of measurement noise.

Usually unknown, model parameters such as heat transfer coefficients and reaction kinetic constants are either estimated offline from test data or on-line using an extended Kalman Filter (EKF) as described by A. Tadayyon and S. Rohani (2001). In a typical application, the process model is made up of between 10 and 100 differential and algebraic equations.

5.3.2 LINEAR EMPIRICAL MODELS

Conventionally, models used in MPC applications are identified through a series of step tests. In some cases, Pseudo Binary Random Sequence (PBRS) tests are used and impulse response coefficients are fitted through least squares or through ridge regression as described by Cutler and Yocum (1991). In most cases, input channels are perturbed one at a time, leading to SISO identification. While this practice is simple and easy to implement, it emphasises the accuracy of individual SISO models and may not yield a multivariable model of required accuracy. Implementing a controller designed with such a model can lead to poor closed-loop performance and instability.

One can experience the same problem with multiple input single output (MISO)/MIMO identification, as long as perturbations introduced to various input channels are independently designed. This is because, in a highly interactive process, gain directionality of the process causes the responses of output channels to exhibit strong correlation, even to extreme co-linearity. This can lead to problems like poor signal-to-noise ratio and strong bias in the low gain direction as described by Andersen and Kummel (1992).

A MIMO identification algorithm on the other hand fits a single model for all the outputs simultaneously while accounting for any existing correlation. Not only can this lead to an improved identification of the deterministic part, but the stochastic part of the model can potentially be useful in the prediction. The latter is particularly true in designing a model predictive control system for those applications where some of the controlled variables are either not measured or measured with large delays and must be inferred from secondary process measurements for satisfactory control.

Although it may be more convenient for models to appear in other forms, control practitioners usually choose to use linear models in state space form. Continuous time models may be more familiar to people with a classic control background in transfer functions but discrete time models are very convenient for digital computer implementation. Most MPC applications and commercial products use linear empirical models.

The discussion of MPC in state space form has several advantages, including easy generalization to multivariable systems, ease of analysis of closed loop properties and online computation. It should however be noted that transformation from continuous-time to discrete-time models is available as a one line command in most programming languages.

For a stable system a Finite Impulse Response (FIR) model may be derived as an approximation to the discrete-time transfer function. This is done by writing it in the form of a matrix fraction description as below:

$$y_i = \sum_{k=1}^{N_u} H_k^u u_{i-k} + \sum_{k=1}^{N_v} H_k^v v_{i-k} + \sum_{k=1}^{N_w} H_k^w w_{i-k} + \xi_i \qquad \textbf{5.7}$$

Typically the sample time is chosen so that from 30 to 120 co-efficients are required in order to describe the full open loop response.

5.3.3 NONLINEAR EMPIRICAL MODELS

One of the important reasons for MPC's success in industry has been the ability of engineers to construct the required models efficiently from plant tests. Unlike the linear case, however, there is no established method to construct a non-linear model through a plant test. The fact that the solution to the optimal control problem is possibly not convex presents theoretical and computational difficulty.

One the non-linear empirical modelling techniques used is a discrete-time linear model for the state dynamics, with an output equation that includes a linear term summed with a nonlinear term. The nonlinear function is usually found by a neural network. The problem however with neural networks is that they tend to be unreliable when expected to perform outside of the range of their training data.

In order to overcome this problem another feature than has been introduced by people who have decided to take this route is that they use an extended Kalman filter to correct for plant-model mismatch and unmeasured disturbances. The extended Kalman filter provides a bias and gain correction to the model online. The way in which identification is done for non-linear empirical models is that a static non-linear model is superimposed over a linear dynamic model, Pearson, Ogunnaike and Doyle, (1993).

An interesting non-linear empirical model structure is the Volterra kernel, which can be viewed as an immediate high-order extension of the FIR model currently employed in most commercial MPC algorithms for linear control. For identification of the Volterra kernel the condition on the input test signals for asymptotic convergence of the parameters under prediction error minimisation has been established by Koh and Powers, (1985). A stumbling block for

embracing this model type as the choice for general non-linear control problems is the large number of parameters which explodes with the systems input dimension. Volterra models beyond second order therefore seem impractical.

Another way in which industry has chosen to derive such models is to assume that the process input and output can be decomposed into a steady-state portion which obeys a nonlinear static model and a deviation portion that follows a dynamic model. The models are derived from pulse tests on the plant to get the linear portion and neural networks trained on historic data for the nonlinear portion.

5.4   MODEL PREDICTIVE CONTROL TECHNOLOGY

Most industrial MPC developers that have chosen to base their technology on the initial DMC ideas have had numerous problems with regard to limitations on model choices, sub optimal feedback, lack of normal stability and sub optimal or inefficient solution of the dynamic optimisation.

Some algorithms rely on convolution models in the form of impulse or step response models. This can be problematic when controlling a process with varying time constants, with another problem arising from the fact that models of this nature are limited to strictly stable processes. Convolution models also experience problems when it comes to processes with widely varying time constants and in most cases dynamic control of the fast processes are sacrificed in order to keep the length of the model horison reasonable.

Most nonlinearity problems experienced with convolution models may be overcome by using an auto-regressive parametric model form like a state space or ARX model.

For plants that have a total absence of disturbance and measurement information the best assumption that can be made for a stable plant is the use of bias update feedback. This can be improved if the distribution of disturbances can be characterised more carefully because the use of bias update implicitly assumes that there are no stochastic disturbances affecting the state of the system and hence that the measurement is perfect. The two main phenomena that are present in most processes are however process noise and integrators, and because this is known by all MPC practitioners each developer has chosen to implement his own ad hoc solution. It should however be noted that most ad hoc solutions fail in the presence of significant measurement noise.

The route that has not been delved into sufficiently is the use of a stabilising algorithm. Some of the solutions to industrial linear MPC technology lie in the use of infinite prediction and control horizons.

The solution algorithms of most industrial MPC controllers have chosen to take the route of utilising a sub-optimal dynamic optimisation because of the need to linearise. This may be acceptable for high speed processes that require the controller to execute in very small time intervals because it would require the QP to also be solved in every execution but in all other applications this is should not be the case. The significant point is that no industrial developer has yet chosen to exploit the structure of a QP in a dynamic optimisation. One industrial solution does offer a singular value numerical technique in the dynamic optimisation but it would be possible for much larger and faster processes to be handled using a QP.

Model uncertainty is another vast field of model predictive control that requires further investigation. Some developers have decided to monitor model uncertainty and provide estimates with regard to it, yet only one MPC package has incorporated this into its controller design. Most packages rather choose to de-tune the controller in order to gain robustness yet the trade-off one has to undergo in performance is not clear. Determining whether a model is accurate enough for a particular control application will only be fully known when the trade-off is understood and measured.

The major limitations that have been found with identification methods arise around the fact that actual plant data comes in a format that requires close inspection by experienced engineers to recognise proper models. It is also not possible to determine whether sufficient dynamic data has been collected in order to properly represent the process for MPC controller design. This usually leads to the test period for step testing being longer than it actually should be which causes undue losses in production and product specifications in certain instances.

Identification algorithms should undergo testing for statistical accuracy and consistency. This will help in investigating new model validation methods that would allow one to identify if a model is adequate for control of a certain process or determine whether significant deterioration is taking place to models in the online controller. This will help to ensure that maintenance is carried out on the controller subsequent to commissioning. The biggest test yet when it comes to dynamic model identification though would be to properly devise a way to conduct tests for nonlinear MPC.

The next generation nonlinear MPC technology will need to allow for the formulation of non-linear models developed purely from first principle process knowledge and operating data. A continuous time fundamental model will be defined from a graphical representation of the plant. Process test signals should then be used to explore important regions to determine adequacy for control. By combining these two methods one will be able to properly predict plant behaviour in order to control the process.

6. 1-OCTENE MODEL DEVELOPMENT

6.1   INTRODUCTION

When one undertakes an advanced control project it is usually expected that the multivariable controller would be developed based on the operational data that is produced by the plant. With this particular study being conducted remotely with minimal access to the actual plant it was decided that an accurate dynamic model of the plant needed to be developed to allow for testing of the controller.

The sponsors of the project prefer to conduct modelling in the Aspentech Engineering Suite environment. They also preferred the use of a particular set of thermodynamic properties which is unique to this particular process. While awaiting the arrival of the specific thermodynamics it was decided that work would be done in parallel to develop a model in the C++ environment using first principles of chemical engineering.

Once the appropriately specified thermodynamics arrived in the form of an Aspen Plus simulation, the column was simulated initially in steady state and then the Aspen simulation was converted to a dynamic simulation.

Both simulations were tested using similar disturbances to check responses of the models against plant data that was made available at a later stage by the sponsor.

6.2   THE FIRST PRINCIPLES MODEL

The aim of this section of the document is to provide an overview of the first principles model of the plant, the solution technique used and some of the features of the model. The primary objective of this model was that it should explain plant behaviour. The plant model should be adaptive, infer certain parameters that cannot be measured and hence provide key information that is required to explain the dynamics of the control system and the online plant. Whereas the plant model was nonlinear, the controller was designed on linear principles, and thus required continuous adaptation to find effective local linear behaviour.

6.2.1 OBJECTIVES OF THE FIRST PRINCIPLE MODEL

The plant model developed needed to be an accurate representation of the plant in order to be used to test the advanced controller. A DMC controller is a linear controller that requires plant step test data in order to be properly configured. Plant operation personnel are usually reluctant to allow people to conduct step tests on the plant because the plant may go into unstable regions during the test and maximum production would not be achieved during this period. Having an accurate plant model would eliminate the need to do unnecessary step testing on the plant because these tests could be undertaken on the model.

Should the need arise the model would also be used for the purposes of operator training, plant process optimisation, and control system optimisation. It is therefore imperative that the model be of a high fidelity in order to achieve these aims.

6.2.2 REQUIREMENTS TO MEET OBJECTIVES OF THE FIRST PRINCIPLES MODEL

The model should be able to run alongside the process and continuously adapt to any changes being made in the process. During this mode new co-efficients are estimated continuously as new measurements become available.

The model should be able to simulate the process predicting the outputs based on any given inputs. This should be done independently of the real process in a prediction mode. During this stage no adaptation of the model is required.

The model could now be used to predict output responses from input changes which could be used in order to fit linear models of the dynamics.

The model should also be robust such that configurational changes are not difficult to make should they be required.

6.2.3 MODEL STRUCTURE

The model was developed specifically for Sasol's 1-Octene Column as depicted in the figure below:
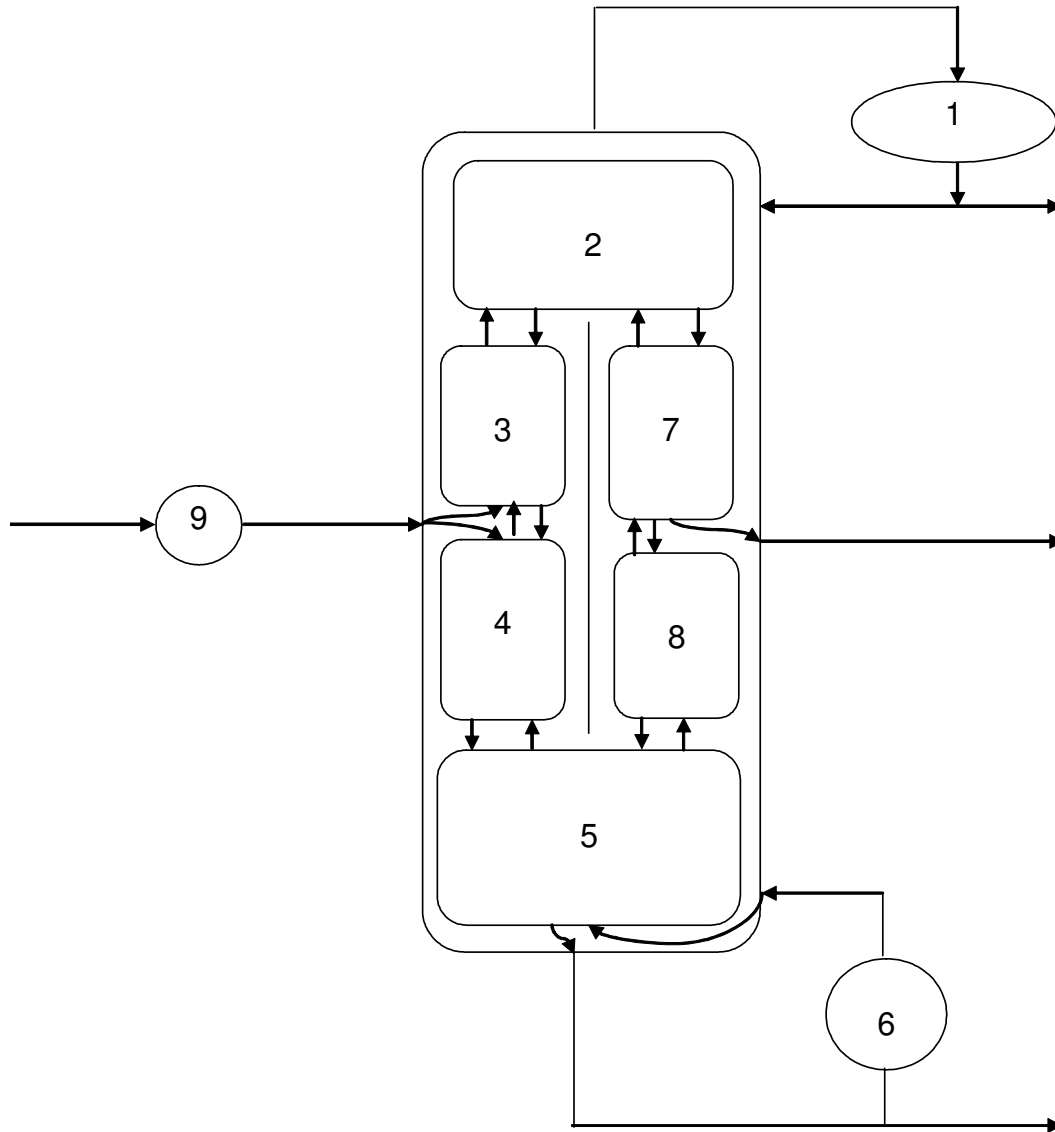
Figure 6.1 Diagrammatic representation of the 1-Octene Column in Secunda

The development of the dynamic model needed to conform to a general structure such that different column representations could easily be accomplished. As depicted in figure 6.1 the column was decomposed into 9 different separation sections each representing a different portion of the column. This method of flowsheet modelling of chemical processes inevitably leads to a set of Differential and Algebraic Equations (DAE), which needs to be solved simultaneously. The algebraic equations usually describe the connections of streams between the column sections whilst the differential equations describe all accumulations in those column sections. Although a solution to this set of equations can be achieved by expanding the

differential equation using the algebraic equations, a loss of readability as a set of ODE's, would exist which would lead to problems when considering changing the column configuration. The relationships are also often implicit, and hence a solution would not be possible.

The 1-Octene Column was broken up into the column sections represented in figure 6.1 in order to facilitate complex modelling of the column. The individual column sections have different inputs made up of a combination of inflows and outflows from other column sections. The feed to the entire column together with the condenser and reboiler duties as well as the Reflux serves as the input to the system with all the other intermediate parameters being calculated.

Each column section is a representation of all the trays that are contained in that section.
Section 1: Total condenser
Section 2: 24 Trays with a spacing of 400mm, weir height of 35mm and hole area of
0.738 m^2
Section 3: 11 Trays with a spacing of 450mm and a weir height of 35mm and hole area
of 0.351 m^2
Section 4: 18 Trays with a spacing of 500mm and a weir height of 50mm and a hole area
of 0.431 m^2
Section 5: 32 Trays with a spacing of 450mm and a weir height of 40mm and a hole area
of 0.923 m^2
Section 6: Kettle type reboiler
Section 7: 15 Trays with a spacing of 450mm and a weir height of 50mm and a hole area
of 0.351 m^2
Section 8: 14 Trays with a spacing of 500mm and a weir height of 50mm and a hole area
of 0.431 m^2
Section 9: Feed Preheater

The trays are numbered from the bottom of the column, with a liquid feed at its bubble point entering on tray 50 which is in the partitioned section of the column. The side draw is taken from tray 47 which is also in the partitioned part of the column. The design pressure of the column is 4 bar(g) and the design temperature is 235°C. Feed to the column is at 100kPa(g). The pressure drop over the entire column is 40 kPa with an operating temperature ranging from a maximum of 188°C to a minimum of 80°C. A total hold-up of 3.5m^3 is available in the sump of the column.

For modelling of the column the component set was reduced to 10 components that represented over 85% of the composition of the actual feed.

The components selected with their boiling points were as follows:

1. 1-heptene   93.64 ^{o}C
2. Toluene   110.63 ^{o}C
3. 3 m heptane   118.93 ^{o}C
4. 1-Octene   121.29 ^{o}C
5. n-Octane   125.68 ^{o}C
6. 2-Hexanone   127.55 ^{o}C
7. Ethyl benzene 136.2 ^{o}C
8. 1-nonene   146.87 ^{o}C
9. 1-decene   170.6 ^{o}C
10. 1-undecene   192.67 ^{o}C

The number of species considered is not necessarily restricted to these 10 components and can be expanded should the need for greater accuracy be required. The column model represented in diagram 6.1 has nine cells with each representing a varying number of stages. The combination of all nine cells represents the 1-Octene column for modelling purposes.

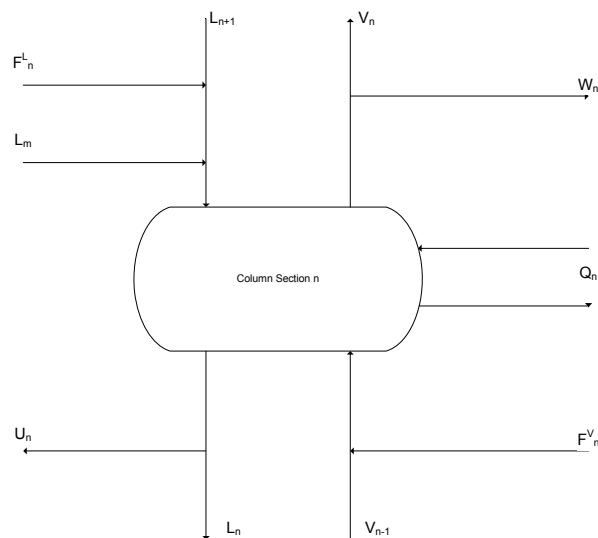The modelling of the overall column was carried out as follows:

Figure 6.2 Representation of a single stage

Phase equilibria, material balances summation equations and enthalpy balances were carried out in order to derive the appropriate set equations to represent the system. These equations are represented below:

The first equation developed is the Mass balance over stage n:

$$\frac{d(M_n)}{dt} = L_{n+1} + V_{n-1} + F_n^L + F_n^V + L_m - (U_n + L_n) - (V_n + W_n) \qquad n = 1,...,NT$$

6.1

Component balance over stage n:

$$\frac{d(M_n X_{n,i})}{dt} = L_{n+1}X_{n+1,i} + V_{n-1}Y_{n-1,i} + F_n^L Z_{n,i}^{LF} + F_n^V Z_{n,i}^{VF} + L_m X_{m,i} - (U_n + L_n)X_{n,i} - (V_n + W_n)Y_{n,i} \qquad i = 1,..,NC \quad n = 1,..,NT$$

6.2

Equilibrium relationship:

$$Y_{n,i} = K_{n,i}X_{n,i} \quad n = 1,..,NT \quad i = 1,..,NC$$

6.3

Summation constraints:

$$\sum_{i=1}^{NC} K_{n,i}X_{n,i} - 1 = 0 \quad n - 1,..,NT$$

6.4

Energy Balance over stage n:

$$\frac{d(M_n \hat{U}_n)}{dt} = L_{n+1}h_{n+1} + V_{n-1}H_{n-1} + F_n^L h_n^{LF} + F_n^{VF}H_n^{VF} + L_m h_m - (U_n + L_n)h_n - (V_n + W_n)H_n + Q_n \quad n = 1,..,NT$$

6.5

Stage hydraulics (Francis Weir formula):

$$L_j = 3.33 L_{wj}(h_{ow})_j^{3/2}$$

6.6

Where:

F_n^L Liquid to feed stage n

F_n^V Vapour feed to stage n

h_n Enthalpy of liquid leaving stage n

H_n Enthalpy of vapour leaving stage n

h_n^{LF} Enthalpy of liquid feed to stage n

H^{VF}_n Enthalpy of vapour feed to stage n

h_{ow} liquid height on weir

$K_{i,j}$ Equilibrium constant of component i on stage j

L_m Liquid feed to stage n coming from remote stage m

L_n Liquid flowrate leaving stage n

L_w Weir Length

M_j Moles of liquid retained in stage j

NC   Number of components

Q_n Heat added or extracted from stage n

t   Time

U_n liquid lateral extraction from stage n

$\bar{U}_n$ Internal energy of liquid retained on stage n

V_n Vapour leaving stage n

W_n vapour lateral stream drained from stage n

$X_{j,i}$ mol fraction of i in liquid phase leaving stage j

$Y_{j,i}$ mol fraction of i in vapour phase leaving stage j

$Z^{LF}_{n,i}$ mol fraction of i in liquid feed to stage n

$Z^{VF}_{n,i}$ mol fraction of i in vapour feed to stage n

The calculation of physical properties for each component was done in the model. All equations used to describe the physical properties of the components in the system were functions of temperature and pressure. The pure component data was acquired from Danner and Daubert *(1989)*. The assumption of ideality allowed the use of K-values to describe the vapour-liquid equilibrium, thus avoiding the need for interaction parameters. The column was broken up into elements as described in fig 6.1, with streams connecting the elements. Adiabatic operation of the column is assumed. The dynamics of the reboiler and overhead condenser are neglected.

The volumetric hold-up is held constant by manipulating the top distillate and bottoms product flowrate respectively. The dynamic changes in the internal energy of the liquid retained in each tray are negligible compared to the effects of latent heats. The dynamic changes on internal energy are significantly faster than the total and component hold-ups which implies that equation 6.5 may be written as an algebraic equation.

The liquid from section 2 to sections 3 and 7 of figure 6.1 are fixed at a ratio in the model with values taken from the tray hydraulic design data provided by Sasol. The vapour flow from section 5 to sections 4 and 6 are also fixed in the model.

The inside-out method outlined in Seader and Henley (1998) was used in order to arrive at a solution for the overall column. Due to the large number of stages in the 1-Octene column it was decided to use a lumped parameter modelling technique to solve for intermediate flows. Each of the column sections represented in figure 6.1 were solved using the lumped parameter method described by Edminster (1961). This is an extension to the Kremser group method for absorption and stripping as described by Kremser(1930).

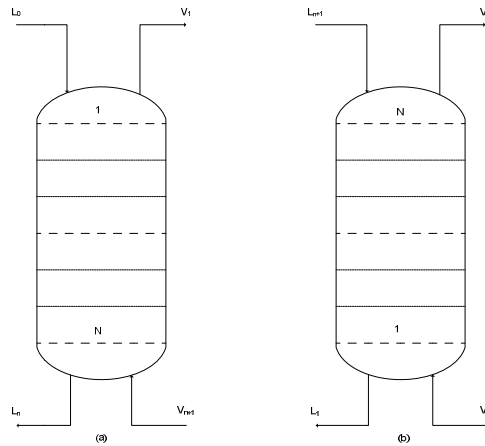Figure 6.3 Countercurrent cascades of N adiabatic stages of: (a) absorber; (b) stripper

Absorption factor for a given stage and component is given by:

$$A_{i,n} = \frac{L_{i,n}}{K_{i,n} V_{i,n}}$$

6.7

Stripping factor for a given stage and component is given by:

$$S_{i,n} = \frac{1}{A} = \frac{K_{i,n} V_{i,n}}{L_{i,n}}$$

6.8

Recovery fraction for absorption is:

$$\emptyset_A = \frac{A_e - 1}{A_e^{N+1} - 1}$$

6.9

Recovery fraction for stripping is:

$$\emptyset_s = \frac{S_e - 1}{S_e^{N+1} - 1}$$

6.10

Total balance in the absorber:

$$y_{i,1} V_1 = y_{i,n+1} \emptyset_A + x_{i,0} L_0 (1 - \emptyset_s)$$
6.11

Total balance in the stripper:

$$x_{i,1} L_1 = x_{i,n+1} L_{n+1} \emptyset_s + y_{i,0} V_0 (1 - \emptyset_A)$$
6.12

Where:

$A_{i,n}$ Absorption factor for component i on stage n

$S_{i,n}$ Stripping factor for component I on stage n

A_e, S_e Effective absorption and stripping factors respectively

Φ_A, Φ_S Recovery factor for absorption and stripping respectively

The overall solution method for the model described as the first principles model for the 1-Octene column was thus a combination of two methods with the lumped parameter method providing intermediate values for the inside-out method.

The model also requires other information in order to properly initialise at a realistic starting point. If it is not started off with these conditions, data from the end of the previous run is used as a starting point. This information includes initial values for compositions and flows of exit streams from the elements. The values used to initialise the model were obtained from mass balance data used to design the 1-Octene column. This was provided by SASOL. A full mass balance for the system has not been presented due to the intellectual property sensitivity of the actual data. A comprehensive set of operational data was also collected from the SASOL operational data system (ODS) system. This was used to view the different regimes that the column operates under. This data has also been omitted due to intellectual property.

The modelling that was done in C++ is not as rigorous as the one undertaken in Aspen due to the fact that a lumped parameter model provided intermediate calculation for flows in the column. These calculations assume adiabatic conditions which does not account for heat losses to the system, which is a factor in dividing wall columns.

6.3   THE ASPEN™ SIMULATED MODEL

The aim of this part of the document is to provide an overview of the ASPEN simulated model of the plant, the solution techniques employed and some of the features of the model. The primary objective of this model is that it should explain plant behaviour. The simulation engine is also very rigorous which allows one to view all the column variables with the resolution detail being defined by the user.

6.3.1   OBJECTIVES OF THE ASPEN™ SIMULATION

The objectives of the Aspen simulations was to give a more accurate account of the 1-Octene column. The reason for developing two models to meet identical objectives was motivated by the availability of the SASOL Aspen Plus simulation, which was used for design of the column. The C++ model lent itself to the development of the control algorithm as they were both created and integrated in the same environment. The Aspen Dynamics model was not directly linked to the controller so testing was done by manually transferring values from the controller to the simulation and vice versa.

REQUIREMENTS TO MEET OBJECTIVES ASPEN™ SIMULATED MODEL

The model should be able to simulate the process predicting the outputs based on any set of given inputs. It is crucial that the simulation model used to analyse the 1-Octene column is fully understood, particularly the way in which it represents the physical and chemical processes relevant for the column. This is because without knowledge of both the 1-Octene column and the model used to simulate it, it is not possible to correctly interpret the discrepancies between the measured data and the simulation outputs.

Model validation is necessary. This will ensure that the predicted output responses can be used to fit initial linear models of the dynamics.

6.3.3 MODEL STRUCTURE

The 1-Octene dividing wall column is a highly coupled distillation system which requires special attention when simulating. There are three possible column types that may be used in Aspen Plus to model this system. These are the RadFrac, RateFrac and MultiFrac column blocks available in Aspen Plus.

The RadFrac block is a rigorous modelling block that can be used to simulate different types of multistage separations. The method used in this block is based on a rigorous equilibrium stage model. It also includes functionality that allows for pumparounds leaving any stage and returning to any stage. This function block can have any number of stages, sidedraws, interstage heaters and coolers, decanters and pumparounds. The mathematical methods used for solution of the RadFrac functional block are the inside-out and Napthali-Sandholm methods.

The MultiFrac block is also a rigorous modelling block that is used for simulating systems of interlinked multistage fractionation units. This functional block can handle any number of columns each containing any number of stages as well as any number of connections between columns or within each column. It is the ideal choice for handling complex operations. The solution is faster using this block but it does not allow rigorous 3-phase calculations. It also cannot be used in Aspen Dynamics which is one of the aims of this study.

The RateFrac block is a rate-based model which incorporates rigorous procedures for treating component coupling effects in multicomponent mass transfer. The number of equations for a rate-based model is much greater than for an equilibrium based model because separate balances are needed for each of the two phases. Rate based models are also affected by the geometry of the column internals as described by Seader and Henley (1998). Correlations are used to describe mass and heat transfer rates. Tray hydraulics are incorporated into the model to enable prediction of the pressure profile. Equilibrium is assumed at the interface. The computing time is generally an order of magnitude more than for an equilibrium based model.

It was initially decided that the structure of the model should resemble the first principles model and so the option involving four interconnected Radfrac blocks was exercised. This method

involved using four different column sections of different relative sizes in order to represent the 1-Octene column as can be seen in figure 6.4.
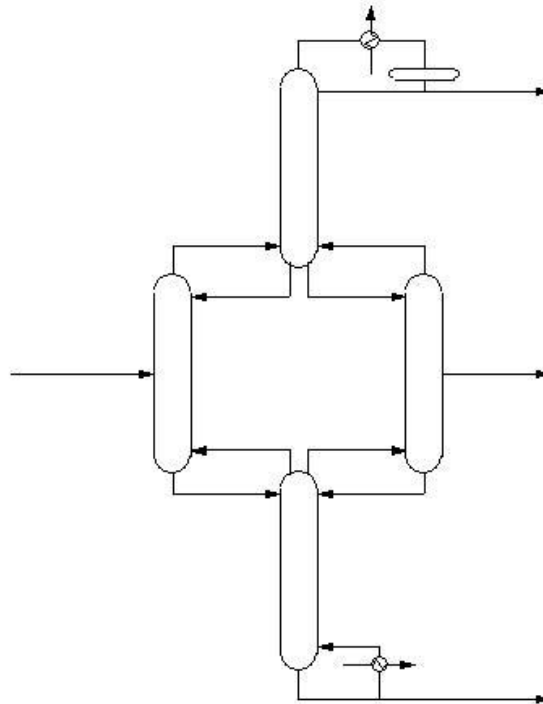

Figure 6.4 Initial model formation used in Aspen Simulations.

The first column type to be used for simulations was the RadFrac block. The flow from one column section to another was difficult to solve in this environment because of the way in which information is populated into the simulation and the order in which the column sections were solved. Prescribed information needs to be fed into the simulation in order to solve. Due to the use of this flowsheet method the simulation is greatly affected by a number of factors including:

- the choice of tear streams
- recycling and convergence methods
- choice of column specification
- balancing the tolerances
- sequencing of the solver

This solution implicitly requires the flows from each column section to be estimated. The solution to these streams is therefore solved by iteration. Rong, Krasalawki and Turunen (2004) investigated thermodynamically equivalent structures and thermally coupled configurations in

relation to traditional distillation configurations. Their results indicate that the thermally coupled configurations have intrinsic uneven distributions of vapour and liquid flows between columns. A distinct feature of a thermally coupled configuration is that it has structural degrees of freedom to re-arrange its column sections. The number of structural degrees of freedom in a thermally coupled configuration is equal to the number of thermal couplings introduced into its traditional distillation configuration.

Subsequent to attempting the flowsheeting approach, the simultaneous approach was attempted using the MultiFrac function block. This method alleviates the necessity to iterate for flows between column sections. The column formation used for this simulation was the Petlyuk column arrangement as indicated in figure 6.5.
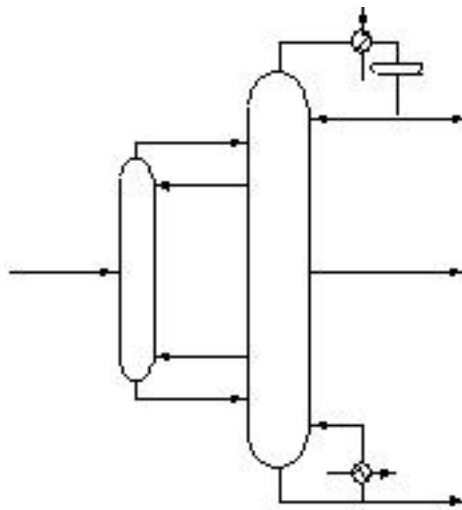

Figure 6.5 Final model formation used in Aspen simulations

Within the MultiFrac function block there are 'sub-column blocks' that are specified. Each of these column sections is individually specified. The number of stages in each column section can be specified and four different stream types may be used to define the column. The external steams are normal Aspen stream types that are used for connectivity to all function blocks. Connecting streams exist only within the MultiFrac function block but external to the column sections. They form the interconnections between the column sections that define the column. The internal streams are the actual liquid or vapour flows between stages of the column sections. Pseudo streams are the streams that store the results of the internal connecting streams of the MultiFrac. The main feature that distinguishes the pseudo streams

from external streams is that they are not used in the mass balance calculations for the function block.

The mathematical solution method for the simultaneous MultiFrac function block is the inside-out algorithm. This algorithm is sufficient for most systems. The main problem experienced with the MultiFrac column type was that it cannot be exported to Aspen Dynamics where further work needs to be conducted. The MultiFrac block generally solves faster but does not allow for rigorous 3-phase calculations.

Knowledge gained from the first two steady state models developed helped to finalise the model structure. It was decided that the final simulation would require the use of RadFrac function blocks rather than the MultiFrac because of the need to conduct all the remaining work in Aspen Dynamics and Custom Modeller. The column arrangement however would not resemble the structure in figure 6.4 but rather the Petlyuk structure in figure 6.5. Fewer streams need to be estimated using the Petlyuk structure as well as the fact that individual tray sizes may be specified for each tray in the RadFrac. This allowed for the middle section of the second column in the Petlyuk setup to be skewed having a thinner centre portion as represented in figure 6.6. The illustrations in figure 6.6 provide an insight into the way in which the 1-Octene column was specified and simulated. Dividing wall columns are not common plant equipment and are thus not specifically catered for in commercial simulation software.

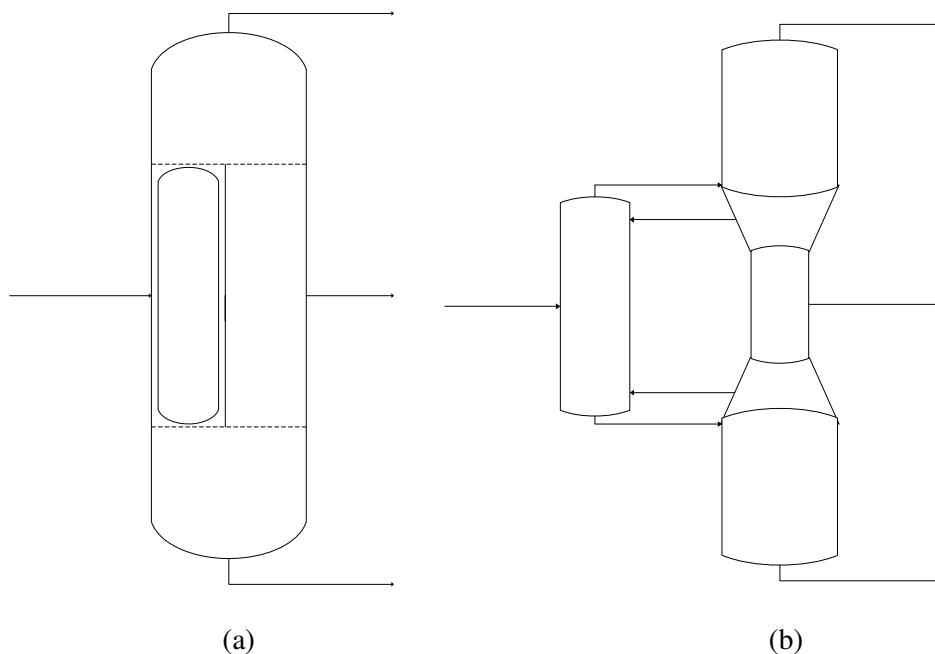(a)   (b)

Figure 6.6 Representation of the way in which tray sizes were specified

There were 51 components used in the specification of the final simulation, 47 of them were found in the PURE11 data bank of Aspen Plus. The normal boiling points for the other four components were user-specified. All the other required pure component properties for these components, eg. Vapour pressure for K-value calculation, were then estimated using the pure component equations of state (PCES). The components used may be found on table 6.1 below:

Table 6.1   List of Components used for simulation

No.	Component ID	Component Name	Formula
1	WATER	WATER	H20
2	NITROGEN	NITROGEN	N2
3	2MPENTE2	2-METHYL-2-PENTENE	C6H12-8
4	HEPTENE1	1-HEPTENE	C7H14-7
5	NHEPTANE	N-HEPTANE	C7H16-1
6	TOLUENE	TOLUENE	C7H8
7	TMCYPENT	USER DEFINED	
8	23DMHEXE	2,3-DIMETHYL-1-HEXENE	C8H16-E1
9	5MHEPTE1	USER DEFINED	
10	3MHEPTAN	3-METHYLHEPTANE	C8H18-3
11	2MHEPTE1	2-METHYL-1-HEPTENE	C8H16-E2
12	T14DMCYH	TRANS-1,4-DIMETHYLCYCLOHEXANE	C8H16-7
13	2EHEXEN1	2-ETHYL-1-HEXENE	C8H16-D1
14	OCTENE1	1-OCTENE	C8H16-16
15	TOCTENE4	TRANS-4-OCTENE	C8H16-D3
16	TOCTENE2	TRANS-2-OCTENE	C8H16-17
17	CONTENE2	CIS-2-OCTENE	C8H16-D7
18	NOCTANE	N-OCTANE	C8H18-1
19	ETHBENZ	ETHYLBENZENE	C8H10-4
20	1ECYHEXE	USER DEFINED	
21	PXYLENE	P-XYLENE	C8H10-3
22	22DMHEPT	2,2-DIMETHYLHEPTANE	C9H20-E1
23	26DMHEPT	2,6-DIMETHYLHEPTANE	C9H20-E2
24	4MOCTANE	4-METHYLOCTANE	C9H20-D3

25	3MOCTANE	3-METHYLOCTANE	C9H20-D2
26	2MOCTEN1	2-METHYL-1-OCTENE	C9H18-D2
27	NONENE1	1-NONENE	C9H18-3
28	C10ENE1	1-DECENE	C10H20-5
29	UNDECEN1	1-UNDECENE	C11H22-2
30	C12ENE1	1-DODECENE	C12H24-2
31	C2ACID	ACETIC-ACID	C2H4O2-1
32	C3ACID	PROPIONIC-ACID	C3H6O2-1
33	IC4ACID	ISOBUTYRIC-ACID	C4H8O2-4
34	NC4ACID	N-BUTYRIC-ACID	C4H8O2-1
35	2MBUT1OL	2-METHYL-1-BUTANOL	C5H12O-2
36	PENTANOL	1-PENTANOL	C5H12O-1
37	IC5ACID	ISOVALERIC-ACID	C5H10O2-D3
38	NC5ACID	N-VALERIC-ACID	C5H10O2-1
39	NMP	N-METHYL-2-PYRROLIDONE	C5H9NO-D2
40	4M2PNTON	METHYL-ISOBUTYL-KETONE	C6H12O-2
41	2MPENTAL	USER DEFINED	
42	3HEXANON	3-HEXANONE	C6H12O
43	HEXANON	2-HEXANONE	C6H12O-D3
44	1HEXANAL	1-HEXANAL	C6H12O-D2
45	2EBUTANOL	2-ETHYL-1-BUTANOL	C6H14O-D2
46	1HEXANOL	1-HEXANOL	C6H14O-1
47	2EC4ACID	2-ETHYL-BUTYRIC-ACID	C6H12O2-D4
48	NC6ACID	N-HEXANOIC-ACID	C6H12O2-D5
49	5M2HEXON	5-METHYL-2-HEXANONE	C7H14O-D10
50	HEPTANON	2-HEPTANONE	C7H14O-D2
51	1HEPTAL	1-HEPTANAL	C7H14O-D1

The simulation environment is usually used for the design of columns with the solution being specified in terms of ideal stages. The number of trays represented in the simulation is hence not identical to the number of stages in the actual 1-Octene Column. The number of stages selected for the simulation was based on the best match for concentration of several

components present in the side draw. The number of stages specified in the prefractionator section of the Petlyuk setup was matched to the equivalent section in the main column with a constant efficiency being specified throughout the column. The actual number of trays in the 1-Octene column is known and thus an implied efficiency of 61% was calculated.

The vapour side draw feeding from the main column to the prefractionation section was set equal to fifty percent of the total vapour available on the tray. This was assumed (fig 6.6a) because there are is an equal number of trays on either side of the wall and the dividing wall is located in the centre of the column hence it is assumed that the vapour distributes evenly to either side of the column. Rigorous 3 phase calculations were carried out on the condenser because water is decanted in this stage.

The reflux flow and internal reflux flow from the chimney tray to the feed side of the column were specified while the distillate and side draw flows were allowed to vary to solve for the 1-Octene purity specifications in the distillate and bottoms streams. A special calculation block was also used to correct for the top and bottom pressures in the prefractionator section from the equivalent stage pressures in the main column.

To establish the proper separation particular care needed to be taken because the 1-Octene column cannot separate components boiling close to 1-Octene such as 2-hexanone. Increasing the loss of 1-Octene to the distillate or the bottoms will eventually not result in a decrease of the concentration of these components in the side draw and hence should not be undertaken.

The feed side of the dividing wall / prefractionator section of the Petlyuk arrangement is critical because a particular amount of rectification needs to be done above the feed tray in order to minimise heavies reaching the top part of the column. These would be carried to the side draw and increase the amount of heavy impurities in the product. Stripping below the feed tray also needs to be properly considered because light and intermediate products could be carried to below the wall which would also cause them to be carried out of the column in the side draw. The light and intermediate products need to be maintained below a particular threshold in the side draw because it adversely affects downstream operations.

Table 6.2. Data comparison of flowrates in Aspen model to plant design data

Stream No.	Flowrates					
	Description	Design	Model	Units	Error	Error %
11-2A	Feed	60522	60522	kg/hr	0	0.0
12-20	Overheads	14114	14825	kg/hr	711	5.0
12-25	Water decant	346.1	435.0	kg/hr	88.9	25.7
12-22	Side draw	13698	14293	kg/hr	595	4.3
12-34	Bottoms	32367	30969	kg/hr	-1398	-4.3
12-19	Reflux	84938	84938	kg/hr	0	0.0
12-21	Reflux to feed side	37482	37482	kg/hr	0	0.0
12-23	Reflux to product side	66130	64169	kg/hr	-1961	-3.0
14-4A	Heavies recycle	1964	2405	kg/hr	441	22.5
12-4	C_{9+}	34331	33374	kg/hr	-957	-2.8

Table 6.3 Data comparison of pressures in Aspen model to plant design data

Block No.	Pressure					
	Description	Design	Model	Units	Error	Error %
VL1201B	Prefrac overheads drum	85	85.0	kPag	0	0.0
VL1201B	Prefrac overheads vapour	85	85.0	kPag	0	0.0

Stream / Block	Description	Design	Model	Units	Error	
VL1201B	Prefrac Bottoms	125.6	125.6	kPag	0	0.0

Table 6.4 Data comparison of temperatures in Aspen model to plant design data

Stream / Block	**Temperatures**				
	Description	Design	Model	Units	Error
11-2A	Cold feed	84.8	84.8	^{o}C	0
12-11	Heated Feed	121.0	121.1	^{o}C	0.1
VL1201B	Distillate / reflux	90.7	92.9	^{o}C	2.2
VL1201B	Overhead vapour	113.8	114.6	^{o}C	0.8
12-21	Liquid at top of wall	131.6	131.1	^{o}C	-0.5
12-22	Side draw	142.7	143.0	^{o}C	0.3
12-34	Bottoms	186.0	187.2	^{o}C	1.2
12-4	Cooled C_{9+}	125.0	123.2	^{o}C	-1.8

Table 6.5 Data comparison of Compositions in Aspen model to plant design data

Stream / Block	**Compositions (Mass Basis)**					Error %
	Description	Design	Model	Units	Error	
11-2A	1-Octene in Feed	10.59	10.59	%	0	0.0
12-20	1-Octene in C_{7-} Overheads	14114	14825	kg/hr	711	5.0

12-25	1-Octene in Water decant	3.1	8.4	ppm	5.3	171.3
12-22	1-Octene in Side draw	45.9	44.0	%	-1.9	-4.2
12-34	1-Octene in Bottoms	866	866	ppm	0	0.0

The steady state model in general has achieved a good fit with respect to the actual plant data. Some components do not behave in exactly the same way as indicated by the design data but in general the required separations are achieved with good matches to the individual stream flows.
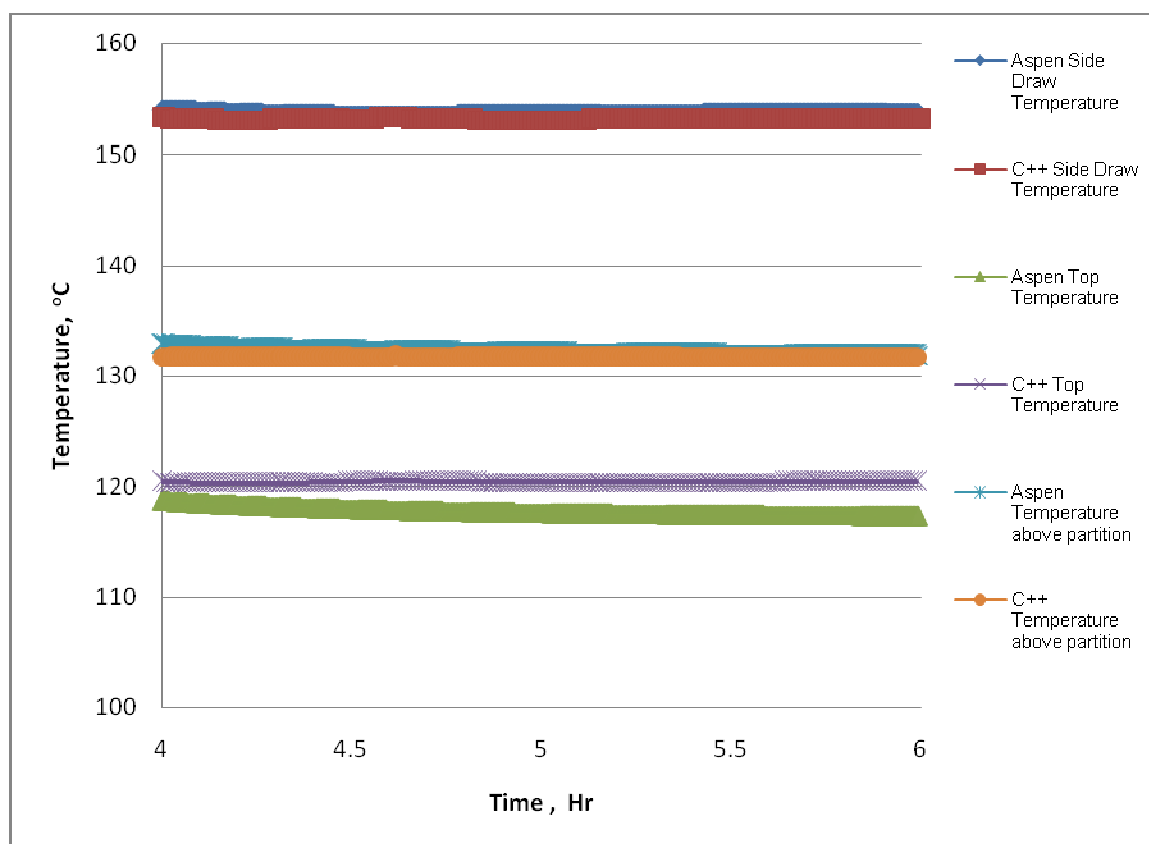
Figure 6.7 Comparison of different model temperatures at Steadystate

Temperature in the 1-Octene column is used as an indication of quality. Both simulations were run at steady state and the results can be seen in figure 6.7. The C++ simulation was setup to explicitly output temperatures and as such a comparison of some of these temperatures was carried.

The side draw is removed from both columns at equivalent stages with the temperatures being closely matched. The temperature prediction for the trayed section just above the partition also matches closely in both models. The temperature at the top of the column varies in the Aspen model while remains constant in the C++ model. This is because the Aspen simulation does rigorous modelling of heat duties in the condenser whereas this was not done in the C++ model. The aspen model manages duty in the overhead condenser which affects temperature at the top of the column. These results show that the models matched one another reasonably at steady state. Both these simulations were run with the same feed rate to each column model.

The design data available from the actual 1-Octene column was used to specify the required column dimensions before the simulation could be exported to Aspen Dynamics.

When an Aspen Dynamics simulation is created, level, pressure and temperature controllers are automatically added to the simulation where deemed appropriate by the program. Each of these controllers has a process variable, Operator set point, and controller output whose values are calculated from the steady-state results of the Aspen Plus simulation. These PID controllers are generally initially populated with generic tuning parameters. All the control loops in the simulation therefore needs to be re-tuned for proper control.

Due to the generic way in which controllers are assigned to an Aspen Dynamics simulation when it is initially imported, a proper control scheme is usually not present. The first action that needs to be performed to simulations that are newly imported to Aspen Dynamics is to properly set up the control scheme.

The PID controls that are currently being used on the 1-Octene column were installed and the individual loops were tuned. Important process considerations as well as particular operations principles that exist in the plant were incorporated into the dynamic model to make the simulation more realistic. Advice from operating personal indicated that the column experienced instability when the duty to the column fluctuated.

In all the simulations, the steam to the reboiler was kept constant. The column has a traditional reflux as well as the internal reflux split which is controlled by a ratio controller. The ratio is important to ensure that no flooding takes place particularly on the feed side of the column. There are no analysers present to check product quality online but there is a big enough temperature gradient in the column to infer product quality using temperature. The quality of the feed is also stable with changes in composition being monitored over time. Changes in feed

quality from upstream operations can be fed forward so that changes to temperature setpoints may be made should they be required. The operating temperatures may vary up to two degrees Celsius. Temperatures in three sections of the column are used for control purposes.

The difference between the overhead temperature together with a temperature close to the top of the column is monitored as shown in figure B2 of Appendix B. The setpoint of these temperatures are set by a differential temperature controller that controls quality at the top of the column. This ensures that 1-Octene is not lost to the overhead product of the column. Temperature control at the bottom of the column is essential to ensure that 1-Octene is not lost in the heavier product from this column. A balance however needs to be maintained between the bottoms temperature and the feed temperature to the column. Other than the obvious relationship between these two temperatures, they are also dependant because heat from the bottom product is used to preheat the feed.

A set of plant data was made available for this study and this was used to validate the model. Step test data was not available to properly check each of the responses of all the controlled variables to changes being made to the manipulated variables independently. The data did contain a fair amount of reasonably sized disturbances and this was used to validate the responses of the model relative actual plant performance.

The dynamic simulations where thus ready for testing of multivariable control strategies.

7. ADVANCED CONTROL OF THE 1-OCTENE COLUMN

7.1 INTRODUCTION

As with any design it is important to begin by establishing all of the important criteria that the final design must satisfy. It is particularly important to understand the nature of the disturbances that are likely to upset the system. Accurate predictions of the feed rate and feed composition disturbances are key elements to eventually developing a robust and workable control structure. When working on an advanced control scheme it Is important to also understand the existing control structure and why it is implemented in the way it is. Reasons for a particular control structure may be very subtle yet critically important to the operability.

The benefits that the advanced process control scheme is expected to deliver can be broadly associated with improving stability of the column, maximising the 1-Octene recovered in the side draw stream and optimising of the energy usage in the column.

7.2 1-OCTENE PREFRACTIONATOR PROCESS DESCRIPTION

An Octene rich feedstock is preheated by the bottoms stream of the column before entering the column on the feed side of the partitioned wall. This column separates the 1-Octene from higher and lower boiling material that are present in the feed. The vapour phase leaving the top of the column contains lower boiling material and is referred to as the C_{7-} stream. This material is condensed in the overhead fin-fan condenser and then flows to the reflux drum where water is decanted, non-condensable gases are sent to the flare while the lighter product is split with some of it being sent back to the column as reflux and the rest being sent downstream for further processing. The 1-Octene rich stream is removed as a side draw from the withdrawal side of the dividing wall.

The source of energy to the column is the reboiler which is heated using medium pressure steam at 2500 kPa. The bottoms stream leaving the column containing the heavier material

referred to as the C_{9+} is split. Part of it passes through a feed preheater and the rest is bypassed around the feed preheater in order to control the feed temperature into the column.

7.3   1-OCTENE PREFRACTIONATOR CONTROL STRATEGY

7.3.1   EXISTING CONTROL STRATEGY

A simplified P&ID showing the basic control system arrangement for the column can be found in Appendix B3.

The flow rate of the feed to the column is measured before it enters into the feed preheater while the valve controlling the feed into the column is located downstream of the heat exchanger. A setpoint for the feed flowrate to the column is decided by the plant operator.

The overall control philosophy is designed to produce a C_8 side draw meeting the 1-Octene recovery and quality specifications. No online analysers were used because purity and recovery is inferred from temperature measurements taken in the column and the side draw flow.

The flow rate of reflux to the column is controlled by a temperature differential controller measuring the temperature difference between the overhead vapour product and the temperature in the upper part of the column above the partition. This differential temperature controller is cascaded to the flow controller on the reflux stream. The scheme is tuned based on the idea that as the differential temperature increases, it is inferred that 1-Octene rich products move up the column, and so the flow of reflux to the column is increased to quench the vapours moving up. While remaining on cascade control the system should react automatically to changes in operating parameters like overhead temperature change, reboiler variations and changes in the flowrate of the side draw.

A temperature differential controller was preferred to a normal temperature controller because the overhead condenser is a fin-fan cooler rather than a normal heat exchanger. Fin-fan coolers are much more affected by sudden changes in ambient conditions. Sudden downpours of rain alter the pressure and temperature of the returning reflux. By using a differential temperature controller the changes in ambient conditions will be compensated for because the overhead vapour will first be affected by the climatic change.

The distillate rate is controlled by the level in the reflux drum which is tuned to achieve averaging control rather than attempting to maintain a particular setpoint.

The second differential temperature controller measures the difference between the overhead vapour and the liquid temperature on the withdrawal side of the partition below the vapour side draw. This differential temperature controller is cascaded to the flow controller on the side draw stream. The tuning of this loop is such that increases in differential temperature reduce the amount of product drawn from the column because it implies that heavier material is moving up the column. The increase in vapour traffic in the column will increase temperatures all the way up the column and will thus be condensed in the overhead product and returned to the column as reflux.

The distribution of the internal reflux to the left and right partition of the column determines the purity of the side draw. The ratio controller should therefore be maintained at the preferred ratio for which it was designed.

The flow of bottom product from the column is manipulated to hold the inventory in the sump. The averaging level control is cascaded to a split range temperature controller that controls the relative amounts of the bottoms product that is passed through the feed preheater and the bypass. A stable optimum feed temperature is achieved using this scheme.

Column pressure is controlled using a split range controller that protects the column from pressure increases by varying the degree of flooding of the tubes in the condenser hence directly adjusting the condensation area with an additional option of flaring inert vapours from the reflux drum should the pressure continue to increase. In cases of decreasing pressure being experienced an automated nitrogen injection system is activated with an additional hot vapour bypass across the condenser directly into the reflux drum.

Heating of the column is set by controlling the flow of medium pressure steam into the reboiler. The control of the reboiler is not self adjusting and is changed manually in accordance with the feed flow to the column. Running on a high heat load increases the purity of each fraction in the column but it is expensive to operate in this manner. A low heat input into the column leads to the deterioration of quality in all fractions from the column. The first indication of this is a decrease in level in the reflux drum followed by a drop in column pressure.

7.3.2 ADVANCED CONTROL STRATEGY

A DMC controller was deployed on the column. The critical controlled variables are kept within a range by utilising the available manipulated variables. The controller takes feed-forward action on disturbance variables that the unit has little or no control over.

7.3.2.1 CONTROLLER OBJECTIVES

- To provide operating stability over a wider operation range
- To respect the unit's process constraints
- To maximise the recovery of 1-Octene in the side draw

7.3.2.2 CONTROLLER SPECIFICATION

The dividing wall column has at steady state five degrees of freedom, which may be selected as manipulated variables:

- reboiler duty (Q)
- reflux
- side draw flow
- Liquid Split
- Vapour Split

There can also be up to four product specifications that may be used as control variables:

- Top Product Purity
- Bottom Product Purity
- Side Draw Purity
- Ratio of light and heavy impurity components in the side stream

Ordinarily all of these variables would be included in the design of the multivariable controller. Due to the nature of the design of a dividing wall column, both sides of the dividing wall are coupled. It is therefore infeasible to independently adjust all of the control variables.

The vapour split occurs as a result of the column internal arrangement and differential pressure on either side of the wall which cannot be independently monitored. The liquid split has therefore been calculated based on this design and is kept constant for all operating conditions.

For the purposes of this study it was decided that there would only be two controlled variables and two manipulated variables included in the advanced controller while all other column variables remain under PID control.

The decision not to include other column variables in the advanced controller was not based solely on the above technical evaluation but also the fact that the 1-Octene dividing wall column aims at recovering 1-Octene in the side draw and does not have as tight product specifications for the top and bottom product.

The purity of the top product leaving the column, the side draw purity as well as the ratio of light and heavy impurity components in the side stream may be inferred by using three different temperature measurements. The temperature measurement taken in the overhead product leaving the column is indicative of the top product purity. The temperature measurements below the reflux and side draw are indicative of light products coming down and heavier products going up the column respectively. These three temperature measurements are combined to calculate the differential temperatures.

The variables selected for the multivariable controller are as follows:

7.3.2.3   CONTROL VARIABLES

1	dTA	Differential temperature between the overhead vapour and the top section of the column
2	dTB	Differential Temperature between the overhead vapour and the liquid temperature on the draw side below the side draw

7.3.2.4   MANIPULATED VARIABLES

1	Reflux	Reflux flow into the top of the column

2	Reboiler duty	Flow rate of Medium Pressure steam to the reboiler

7.3.2.5 DISTURBANCE VARIABLE

1	Feed Flowrate	Flow rate of feed into the column from upstream operations.

7.3.2.6 EXECUTION FREQUENCY

The controller executes every minute.

7.3.2.7 INTERMEDIATE CALCULATIONS

- Differential temperature at the top of the column (dTA)
- Differential temperature for the middle of the column (dTB)
- Calculation of reboiler duty from the Flowrate of steam to the reboiler

An intermediate calculation for the duty of the reboiler will not be required in the advanced controller for the actual 1-Octene column but is used for this study because of the variables required in the dynamic simulation.

7.3.2.8 PROGRAMMING THE MULTIVARIABLE CONTROLLER

The advanced controller implemented aims at driving the column towards a more stable operating range while maximising the amount of 1-Octene being recovered in the column. Selected parts of the code are available in Appendix A.

An initial set of parameters needs to be setup. The program can default to a predefined steady state for initialisation or retain the last set of simulation results as a starting point. The program also allows a new set of conditions to be filled during each time step of the controller. This was done to enable manual feedback of results from the Aspen Dynamics simulation.

The reset function takes the simulation back to the predefined steady state while the step mode allows the simulation to pause after each execution such that feedback may be entered. The number of control moves as well as DMC weights may be entered by the user.

The model is multivariable and non-linear with a mixture of differential and algebraic equations, with state variables, outputs, inputs, associated variables and physical parameters. The output from the model is a set of fitted estimates in real time for state inputs, associated variables, and physical properties. Intermediate calculations need to be carried out during each set of observations.

The result from each iteration needs to be re-interpreted in the code before being sent as final outputs. In some cases the output needs to be clipped due to a constraint. A flowsheet depicting the execution cycle of multivariable controller has been depicted in appendix B5.

Simulation speed may also be altered while running the control model.

7.3.2.9   OTHER CONTROL CONSIDERATIONS

There are no analysers being used for control because the differential temperatures are deemed to be a sufficient measure of quality. Laboratory analysis that is conducted is used to calculate the loss the 1-Octene to the Overheads and Bottoms streams. This however is done once a shift and cannot be compensated for in real time.

The base layer controls that have not been included in the advanced controller are tuned using the Scientific Wild Ass Guess (SWAG) method as described by Cohen and Coon (1953). Instability in these control loops could cause instability throughout the column.

Every loop in the Aspen Dynamics simulation was also tuned using the SWAG method. Regulatory layer controls should always be working at their optimum before advanced control is considered.

7.3.2.10   INTERFACE TO THE CONTROLLER

The first principles model interfaces seamlessly with the advanced controller developed because the entire development of the controller and the model was undertaken in the same programming environment. They are represented as different objects in the same overall program. Figure B-2 in Appendix B is a copy of the user interface created for the model and controller.

Creating an interface with the Aspen Dynamics simulation was not possible. Attempts at creating an interface in the Aspen Custom Modeller environment were undertaken. The vast

differences in the object types and the product specific programming language meant that creating the interface was not possible.

Data was thus manually fed to and from the multivariable controller and the Aspen Dynamics Model.

7.3.2.11   TESTING OF THE ADVANCED CONTROLLER

Both the first principles C++ model and the Aspen Dynamics model were used to test the DMC controller. Performance testing of the advanced controller using the first principles model was relatively seamless. This dynamic model was first step tested to attain the step response models for the controller. Once this was implemented in the controller, various disturbances were imposed on the system to test the control.

The performance testing of the advanced controller in the Aspen Dynamics environment involved running the two programs independently. The Aspen Dynamics simulation was first step tested in order to properly populate the correct models into the controller. The actual test was done manually. The particular disturbance is imposed on the system and the simulation is then run in one minute intervals. One minute intervals were used because they represent the execution frequency of the advanced controller. After each minute the changes in the controlled variables are fed back into the controller which solves for the next set of manipulated variable values. These are then fed back into the simulation. This cycle of events was carried out for the duration of the controller testing.

The testing method for the Aspen Dynamics simulation was thus a highly tedious but necessary process in order to properly test the controller.

8. DISCUSSION AND RESULTS

This thesis has primarily investigated modelling and control of the 1-Octene dividing wall column. The need for this type of investigation rises from the increased use of dynamic modelling as a tool to predict plant behaviour during design, as well as outlining the advantages of using advanced process control in production facilities.

Model detail has varied considerably between the two models that were developed for this study. Controllability and flexibility have been considered in relation to a specific optimal operating point. It can be argued that controllability should be considered at all operating points but the scope of the project dictated that the current operation of the 1-Octene plant should be used as the optimal operating point.

The choice of control structure and controller type plays an important role in plant operation. This thesis has focused on the use of a 2x3 Dynamic Matrix Controller, which is the preferred advanced controller type used in Secunda.

A complete set of steady state plant data was obtained from SASOL for the 1-Octene plant and was entered into the first principles model as the standard set of operating conditions for all the streams. The model was then run in a simulation mode setting all these values as being observed. Once the column model was converged the absorption and stripping rate constants for the plant were set at these values. The operating conditions for the column or column variables would then be calculated using this set of constants.

The model developed in Aspen Dynamics was converged to the operating point of the 1-Octene Plant. Tests were then run in Aspen Dynamics to investigate the response of all variables to step changes.
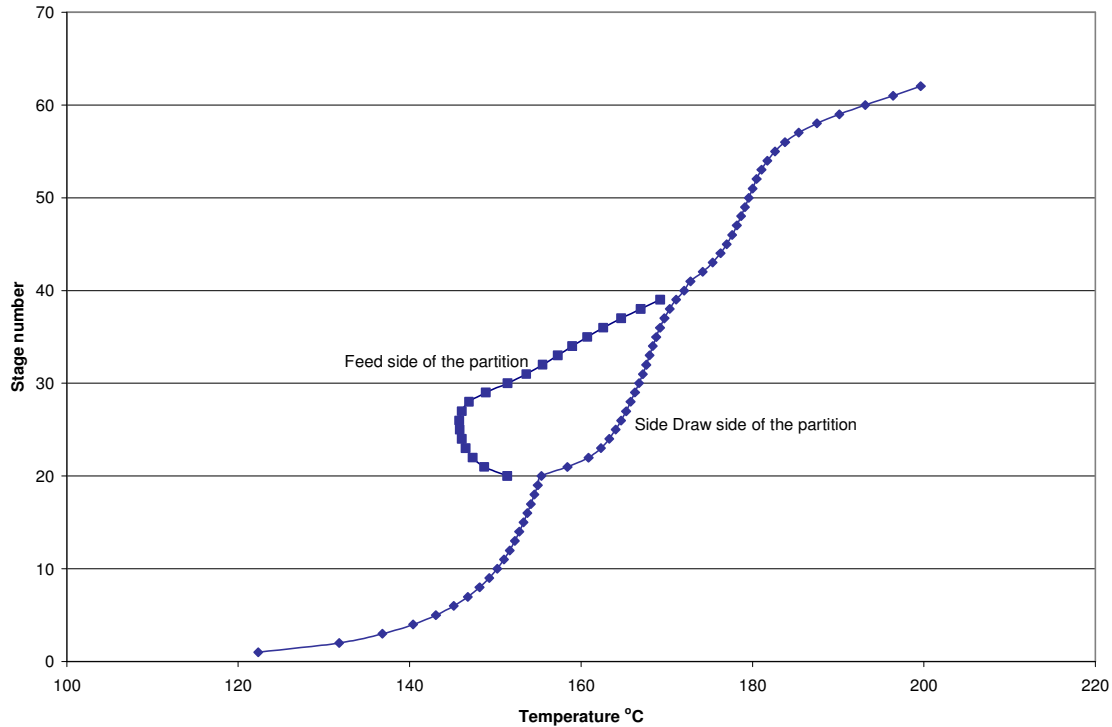
Figure 8.1 Temperature profile of the Column from Aspen Dynamics

Fig 8.1 shows the temperature profile of the column. It should be noted that stages are numbered from the top of the column. The most interesting feature of this plot is that one can clearly see the difference in temperature on either side of the partition.

The temperature difference between the feed side and withdrawal sides of the column is quiet significant and heat transfer across the wall increases the degree of coupling in the column. Significant disturbances in the feed could cause instability in the column.

The results of step testing the models will now be analysed. Step tests were initially conducted on the disturbance variable which is the feed flow rate. Subsequent tests were performed by altering the reflux, side draw rate and reboiler duty. Tests were performed in 5% increments and results obtained show the response of each of the column variables. There are many column variables that represent the total column output in real time some of which remain constant for these tests. Only the relevant trends that showed variable responses are presented.

The sequence that was followed for all variables are as follows:

- 5% Increase
- A second 5% increase
- Three consecutive decreases by 5%
- A final 5% increase

This is the sequence that is followed when stepping variables on the actual plant in order to ensure that sticky valves and other phenomenon on the particular control loop may be identified. It is also done to ensure that the process is returned to its initial condition when step testing is completed.   It is noted however that phenomena such as sticky valves and other loop characteristics would not be seen in these model based tests.

A full set of step tests will first be presented. These results show the response of each critical variable in the simulations. Identical tests were conducted on both the Aspen Dynamics and C++ simulations. Many variables may be incorporated into one plot but the resolution is not sufficient for analysis.
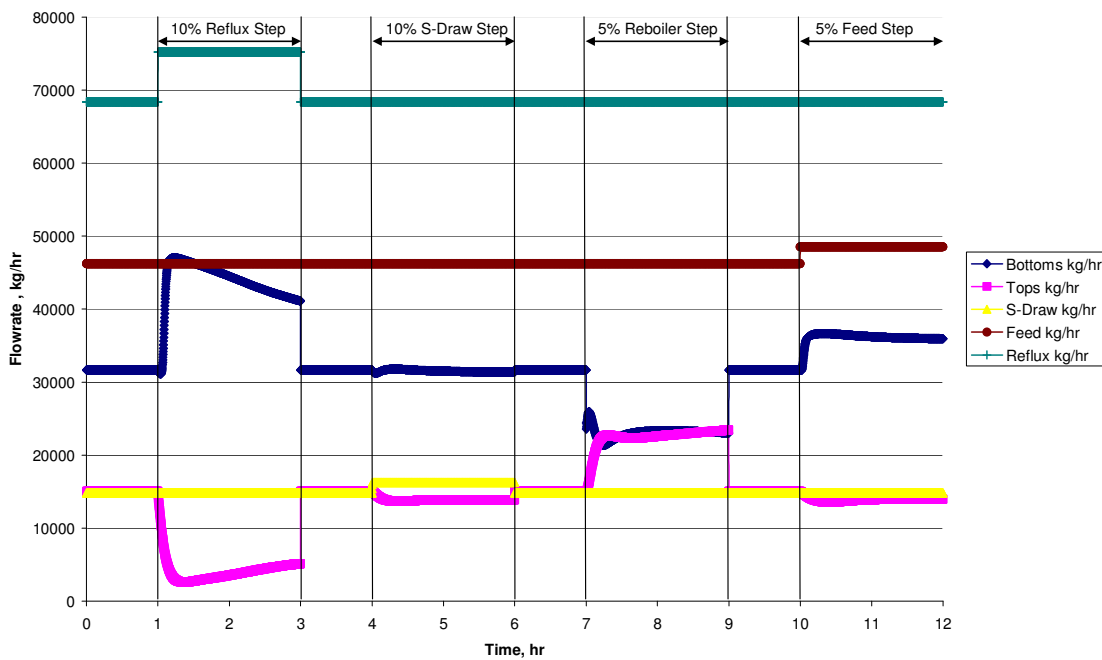
Figure 8.2 Step test responses of flow rates from the Aspen Dynamics model
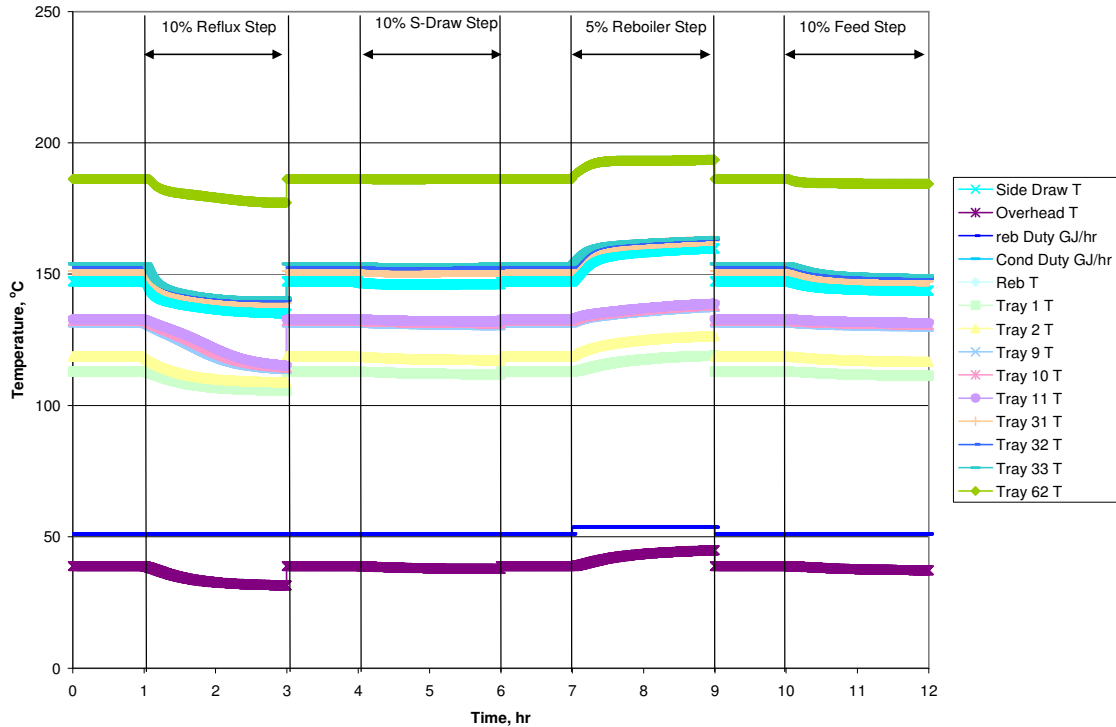
Figure 8.3   Step test responses of temperatures from the Aspen Dynamics model

It is clear from the response in figures 8.2 and 8.3 that reboiler duty and reflux changes have the biggest effect on the profiles all along the column. The Aspen Dynamics simulation performs well with no discontinuities in the results produced. When step sizes are too large simulations tend to reach mathematical limitations which are in keeping with physical limitations of the design, like the drying up of trays.

The resolution of figures 8.2 and 8.3 is limited which makes it difficult to see slight deviations in column profiles due to interaction. Individual plots will be presented discussing the response of each variable to a step change. It is also important to observe the relative difference of the response of each model.   It is for this reason that the plots contain two curves each representing the response of the same variable in the different models.

Temperatures on the feed side of the partition are not critical variables for control and are not shown in these plots. The withdrawal side of the partition is shown because the differential temperature controller uses this for control.
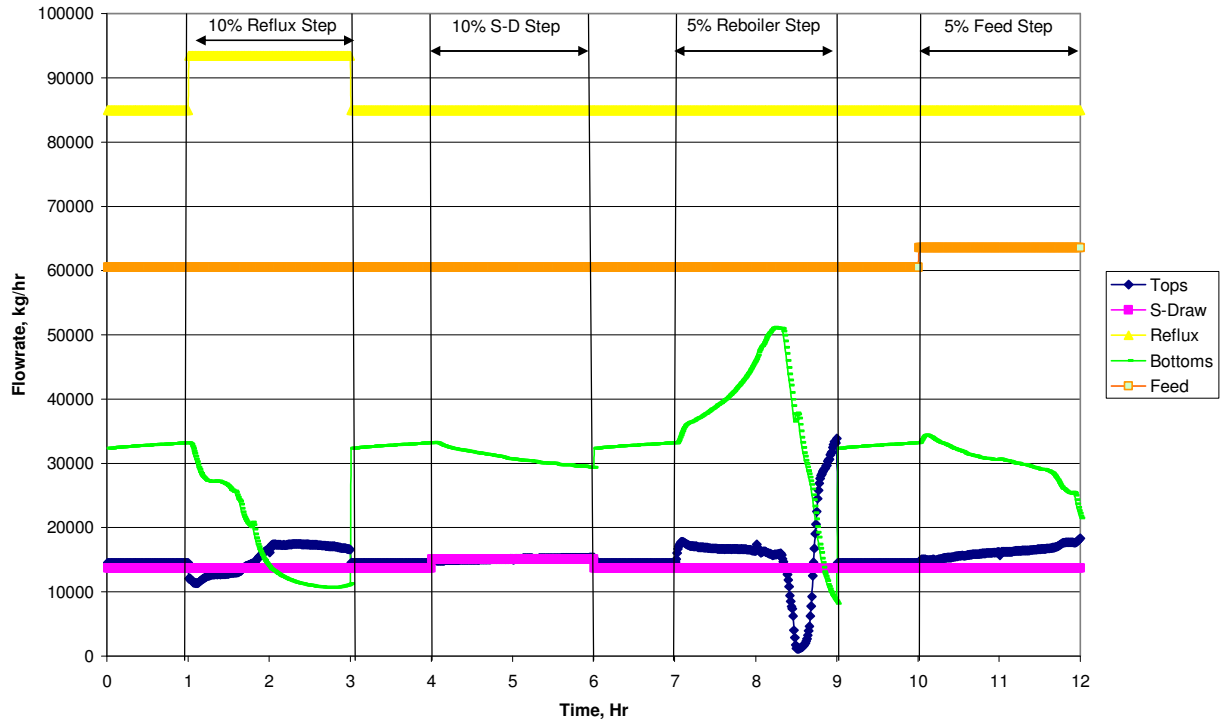
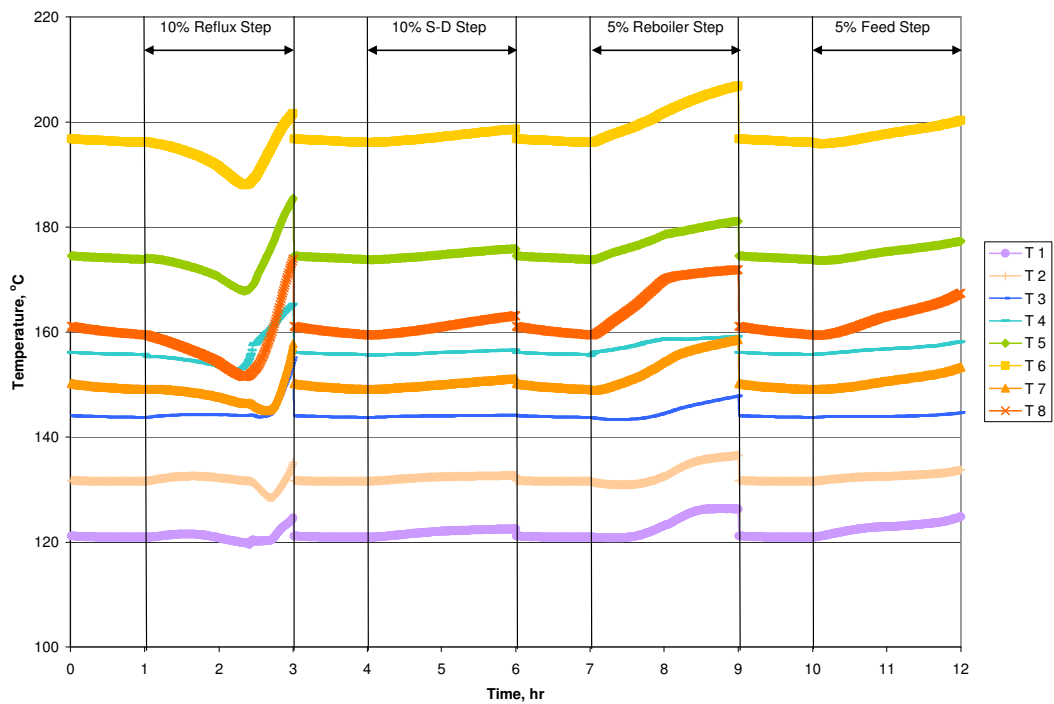Figure 8.4   Step test responses of flowrates from the C++ Model

Figure 8.5   Step test responses of temperatures from the C++ Model

The responses of the variables in the C++ model can be seen in figures 8.4 and 8.5. The labelling on the curves produced from the C++ model are different to those produced in the Aspen Dynamics model.

The C++ model was separated into 9 compartments as represented in figure 6.1. The intermediate flows shown in this figure represent flows within the column and not streams exiting the column. The temperatures are the average temperatures in each compartment, and the flows are the liquid flows emerging from each compartment. A discontinuity can be seen at about 8.5 hours when the reboiler duty was increased. The lumped parameter method used for generating the C++ model is capable of simulating the same set of conditions at steady state but finds limitations in its dynamic responses. The temperatures follow in the opposite direction as compared to the Aspen simulation. The dynamic responses from the C++ model are not indicative of the dynamic behaviour of the 1-Octene column. Discussion of the individual curves from the C++ model will be done when comparing them to the curves generated by the Aspen Dynamics simulation.
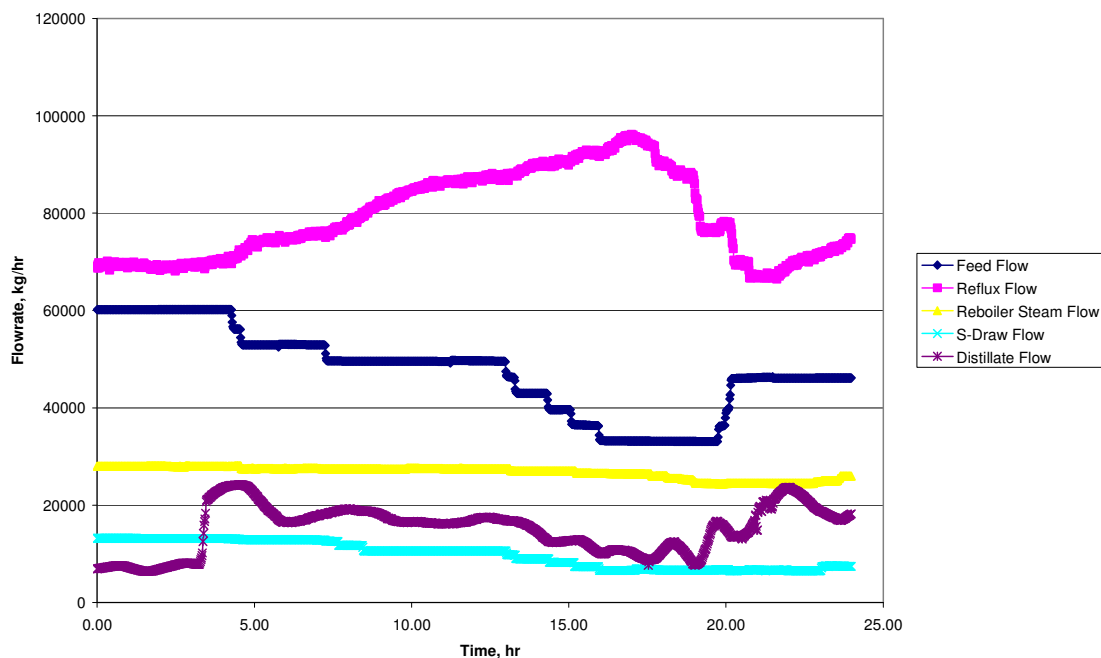

Figure 8.6 A sample of the flows available from the plant data for model validation
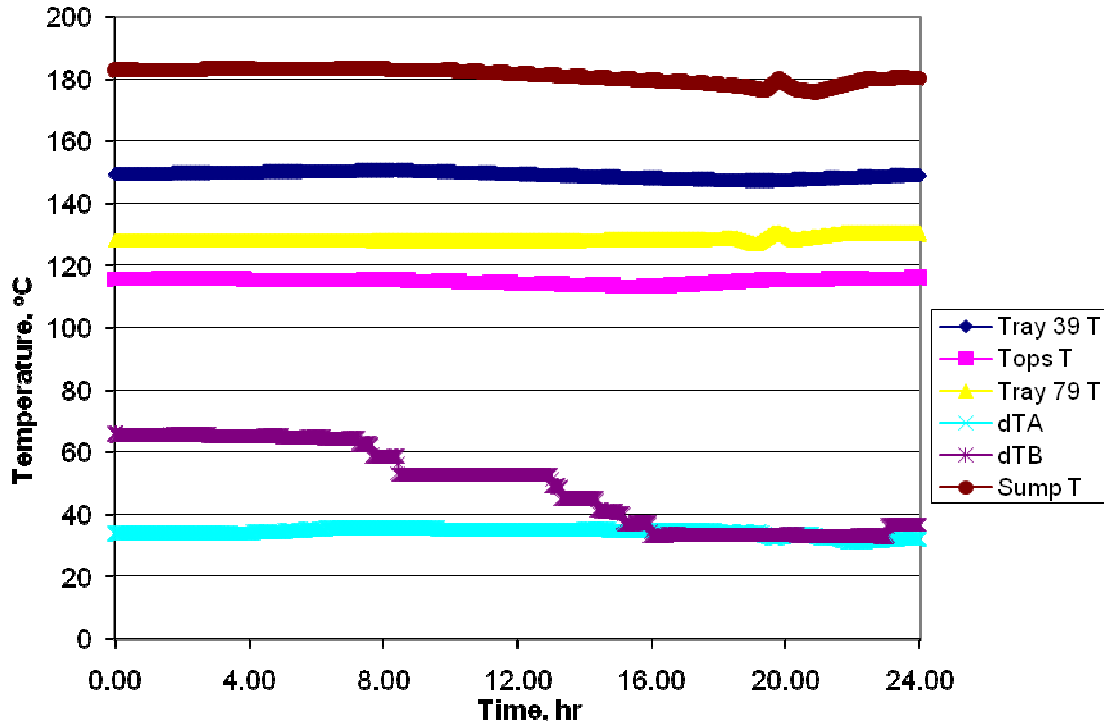
Figure 8.7 A sample of the temperatures available from the plant data for model validation
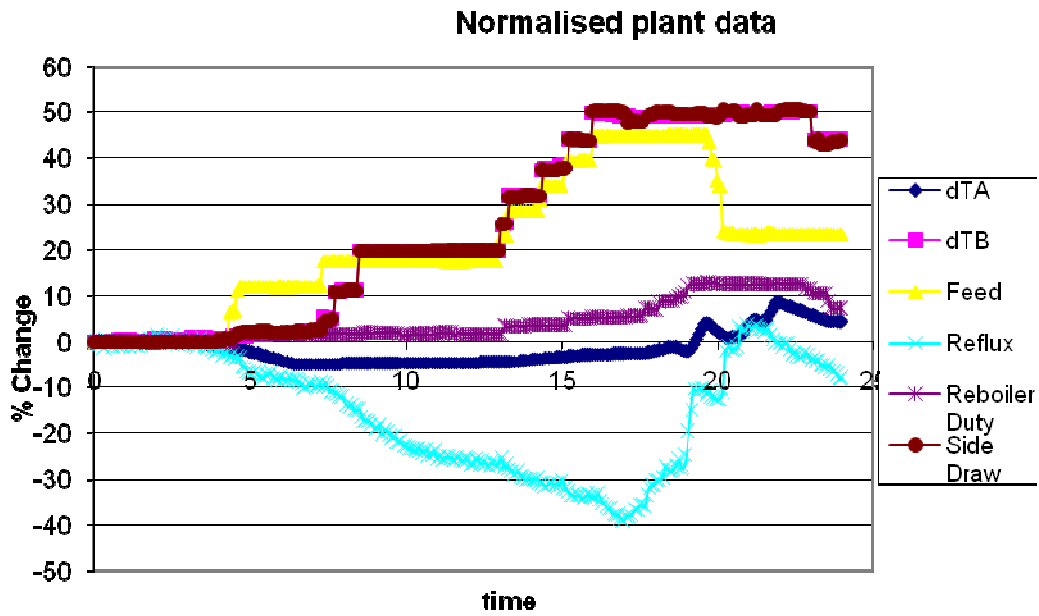

Figure 8.8 Normalised plant data used for model analysis

The available plant data indicated in figures 8.6, 8.7 and 8.8 were used to validate the models. The aspen simulation correlated with the data. The C++ model responses were in certain instances contrary to plant behaviour. The flows and temperatures from the models were checked against the plant data. All of the data was not available in the same form and conversions were needed in order to compare the profiles. Most flows were available as volumetic flowrates. The bulk density in each stream was calculated in order to adequately convert to mass flowrates. The steam flowrate was converted to a duty in order to compare the heat input from the reboiler.

Figure 8.8 should be viewed in context as it is not the response of the column in open loop but rather the response of the column to changes with the existing control system running. It does however assist with understanding the column.

The plots that follow show the relative changes in dTA and dTB in response to the step testing. The steady-state setpoints for these variables were 19.79 and 41.67 ^{o}C respectively. The relative amount that each temperature deviates from 0 in the plots shows the sensitivity of these differential temperatures to the changes in manipulated and disturbance variables.
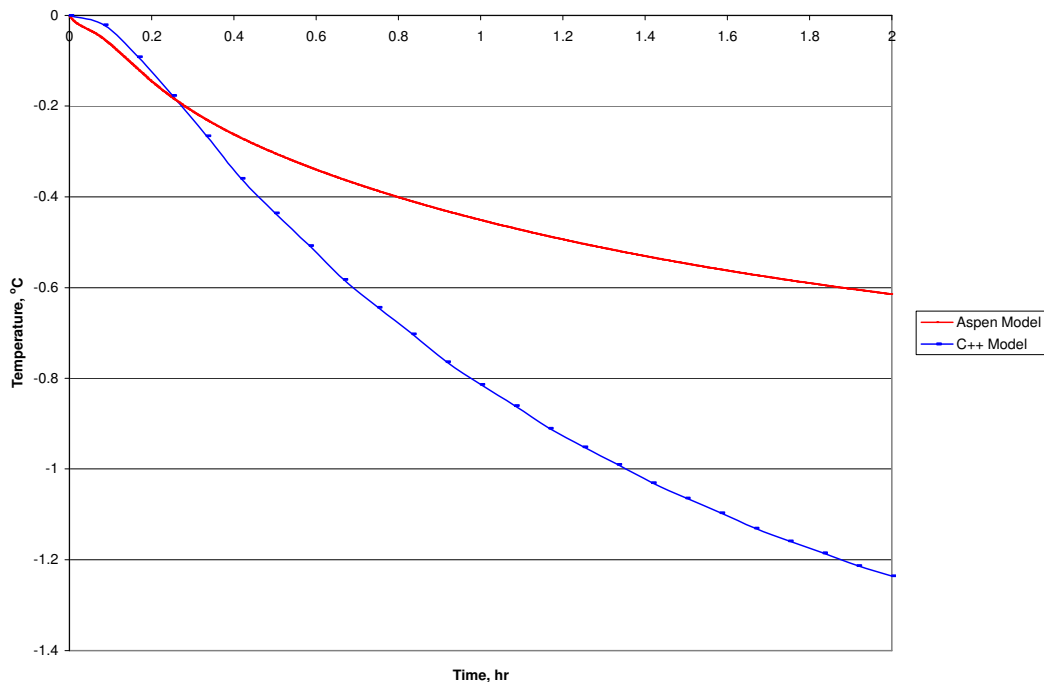

Figure 8.9 Response of dTA to a 5% change in feed flow rate

Figure 8.9 shows the reaction of upper differential temperature to a change the feed flowrate. All other manipulated variables were kept constant during the testing phase. It can be seen that both models are directionally the same with the magnitude of the responses varying due to the different levels of detail contained in each model.
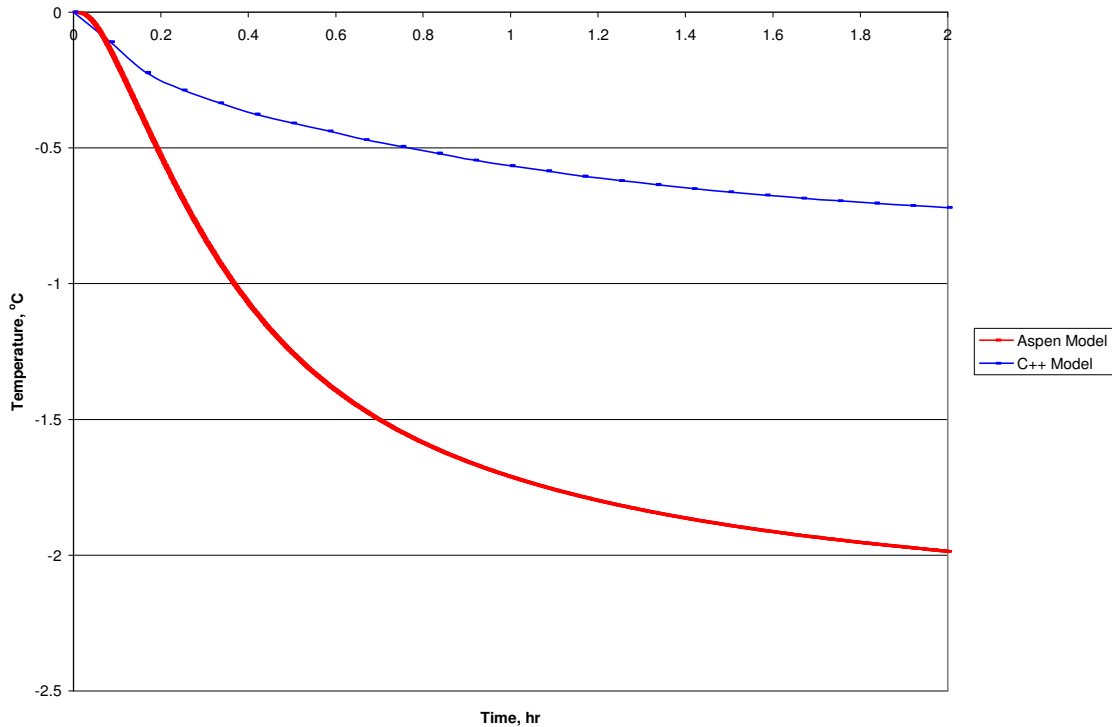

Figure 8.10 Response of dTB to a 5% change in Feed Flowrate

Figure 8.10 shows the reaction of the lower differential temperature to a change feed flowrate. Once again it can be seen that both the models are directionally similar with the magnitude of the responses differing due to the different levels of detail included in each model. The C++ model is a lumped parameter model which uses average temperatures in each column section.

The plant data indicated that changes in feed conditions changes the loading in the column but these disturbances are absorbed by the design. Large variations or instabilities in the column variables are not seen when the feed is changed. The C++ model however does not display this behaviour.

After stepping the feed to the column, which represents the disturbance variable in the advanced controller, the two manipulated variables were stepped. Once again step tests were performed in 5% increments.
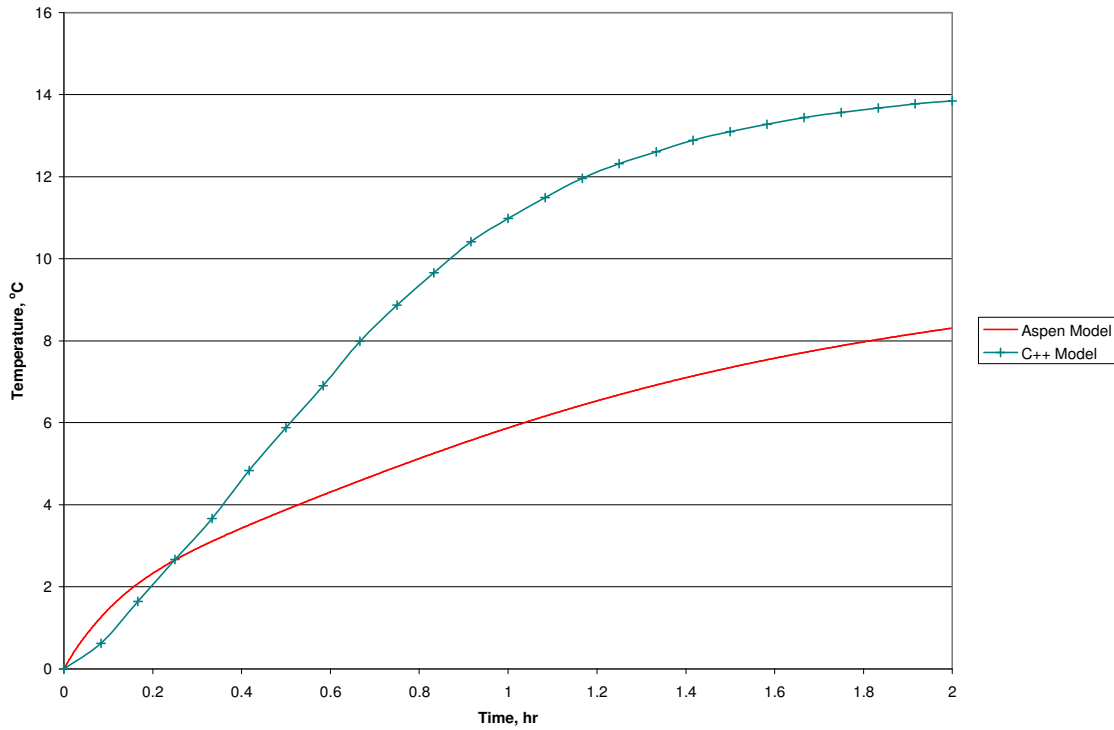

Figure 8.11 Response of dTA to a 5% increase in Reboiler Duty

Figure 8.11 shows how much the upper differential temperature is affected by changes to the duty of the reboiler. Changes in the duty to the reboiler in the simulation are essentially represented in the real plant by changes to the steam flowrate or steam quality to the reboiler. The magnitude of the differential temperature change seen in the column clearly shows that reboiler duty is the most influential manipulated variable that can be used on the column.
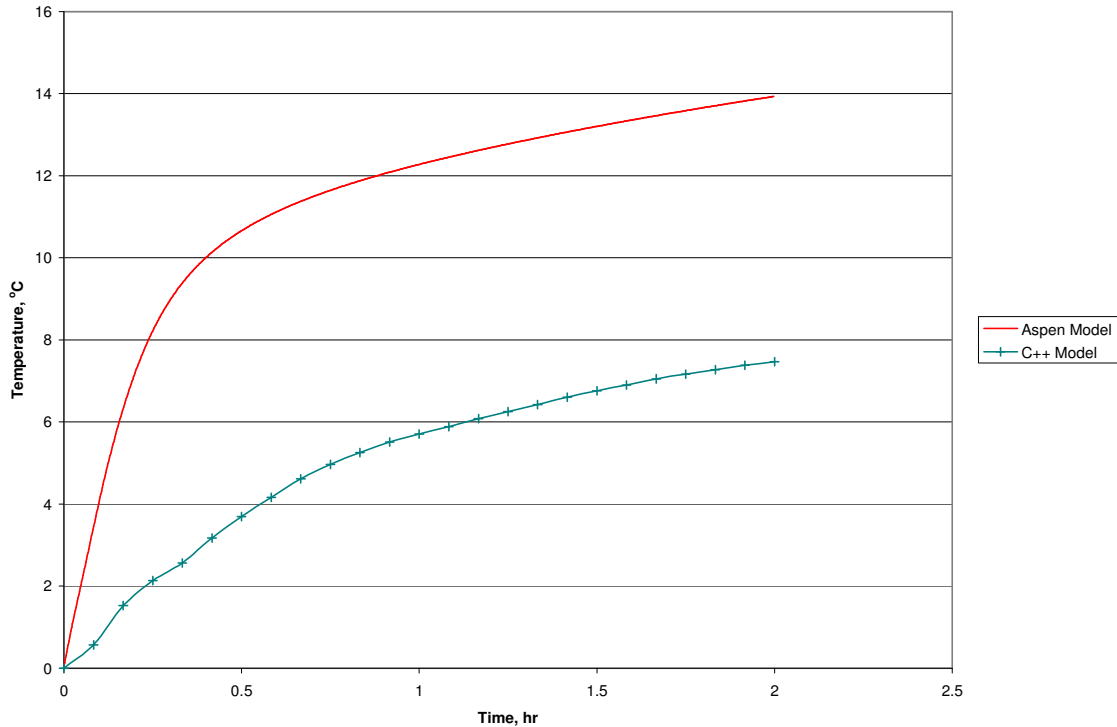
Figure 8.12 Response of dTB to a 5% increase in Reboiler Duty

Once again for the lower differential temperature response in figure 8.12, the strong effect of changes to the heat input to the column can be seen. In relation to figures 8.9 to 8.16, these plots also show that the heat input into the column has the strongest influence on the control of the column.

Plant data show in figure 8.8 also validates that the reboiler duty is the most influential manipulated variable on the column. It also shows that the lower differential temperature is closely coupled to changes in duty to the column as compared to the upper differential temperature. This trend is once again seen in the results from the Aspen Model but not in the C++ model.

The lower sections of the column are obviously more affected by changes to the heat load to the column because these changes propagate from the bottom of the column. The effects usually does not reach the top of the column under normal operation because this would be picked up early and reflux would be used to cool the rising hot vapours and stop heavier products from moving up the column.
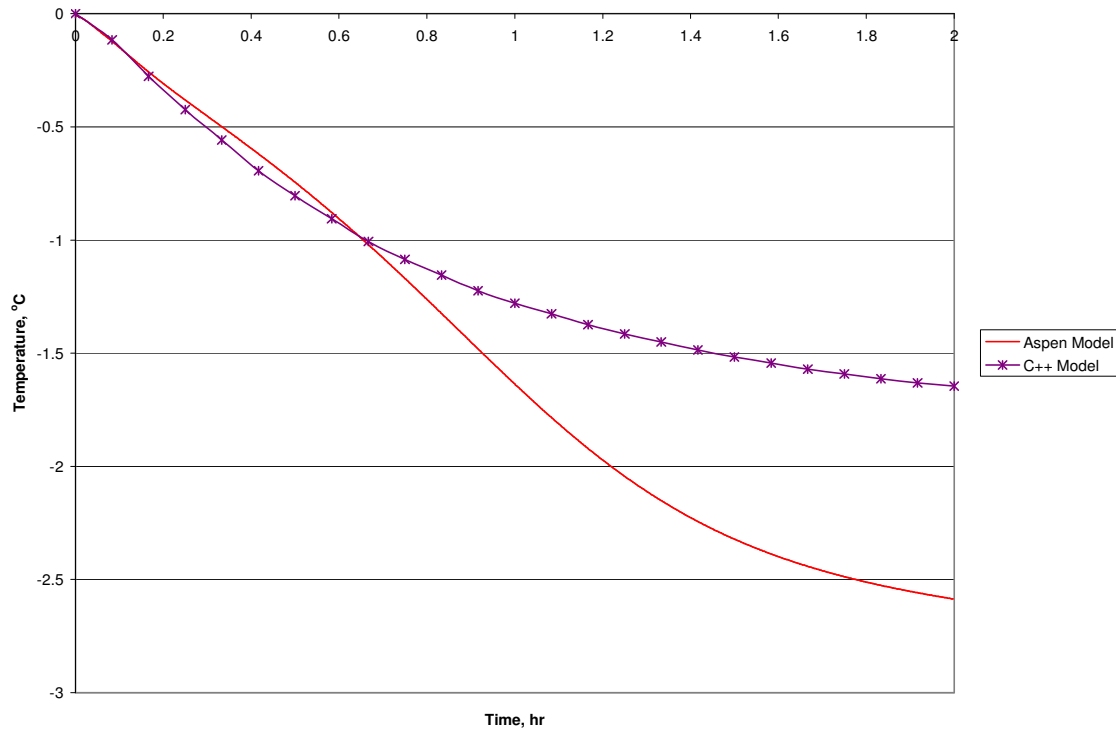
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Figure 8.13 Response of dTA to a 5% change in Reflux Flowrate

Figure 8.13 shows the response of the upper differential temperature to an increase the reflux flow. The Aspen model shows a greater degree of cooling in the upper part of the column as compared to the C++ model. The C++ lumped parameter model uses an average temperature for the upper part of the column as compared to the rigorous Aspen model that takes each tray into account.

As expected there is a decrease in temperature seen at the top of the column when the amount of sub cooled reflux is increased. Both models are directionally correct and they display the same characteristics as the actual column.
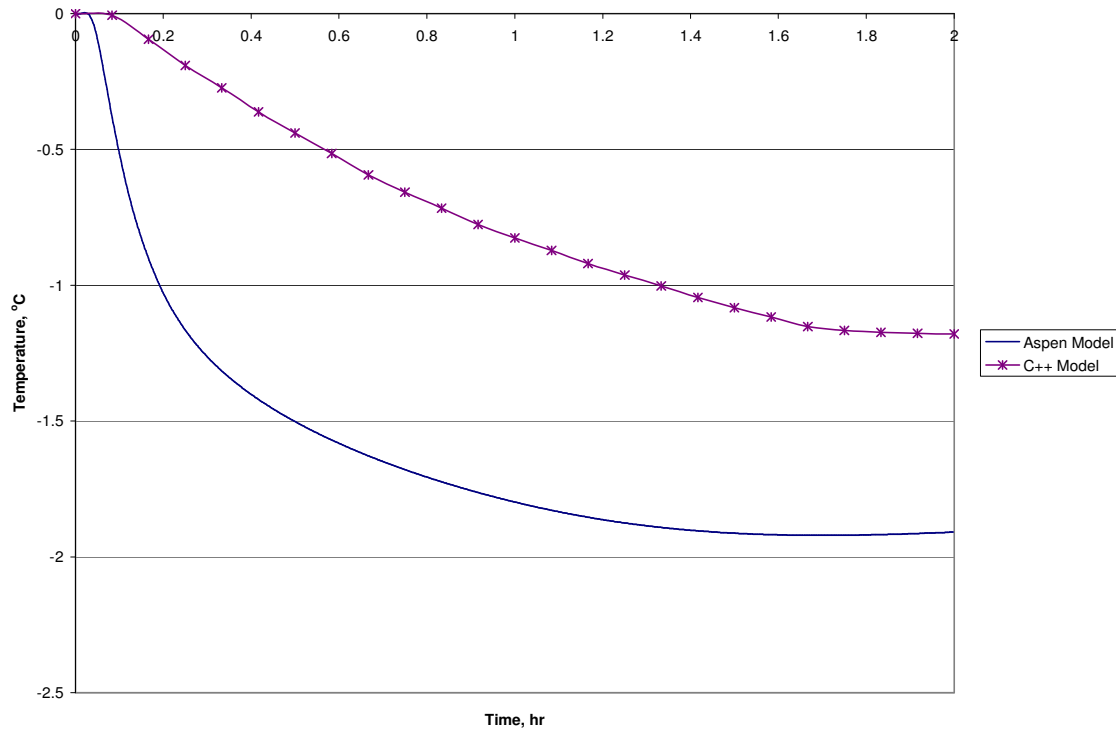
Figure 8.14 Response of dTB to a 5% change in Reflux Flowrate

The effect that an increase in reflux flow to the column has on the lower differential temperature measurement can be seen in figure 8.13. Both models show a decrease in temperatures. The Aspen model once again shows a greater degree of cooling because of the rigorous temperature calculations performed on each tray as compared to the C++ lumped parameter model that calculates average temperatures for each column section as depicted in fig 6.1.

Both models are directionally correct showing a decrease in the differential temperature in the column. The magnitude of the lower differential temperature measurement is smaller than that of the upper differential temperature measurement. This is expected because the subcooled reflux is introduced into the column at the top with it being coolest when it enters but is heated by the rising vapours.

The response of both the Aspen and C++ models to changes in reflux is in keeping with the trends seen in the plant data. The heat to the column does not adjust to the increased cooling during this step test because the effect of a change in reflux is being investigated. The additional liquid load moving down the column lowers the temperature at the top of the column.

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The rate at which the main side product leaves the column has also been known to have an effect on the temperatures in the column and as such an investigation into the effect of Side Draw rate on the upper and lower differential temperature measurements was conducted. The results can be seen in figures 8.15 and 8.16 respectively.
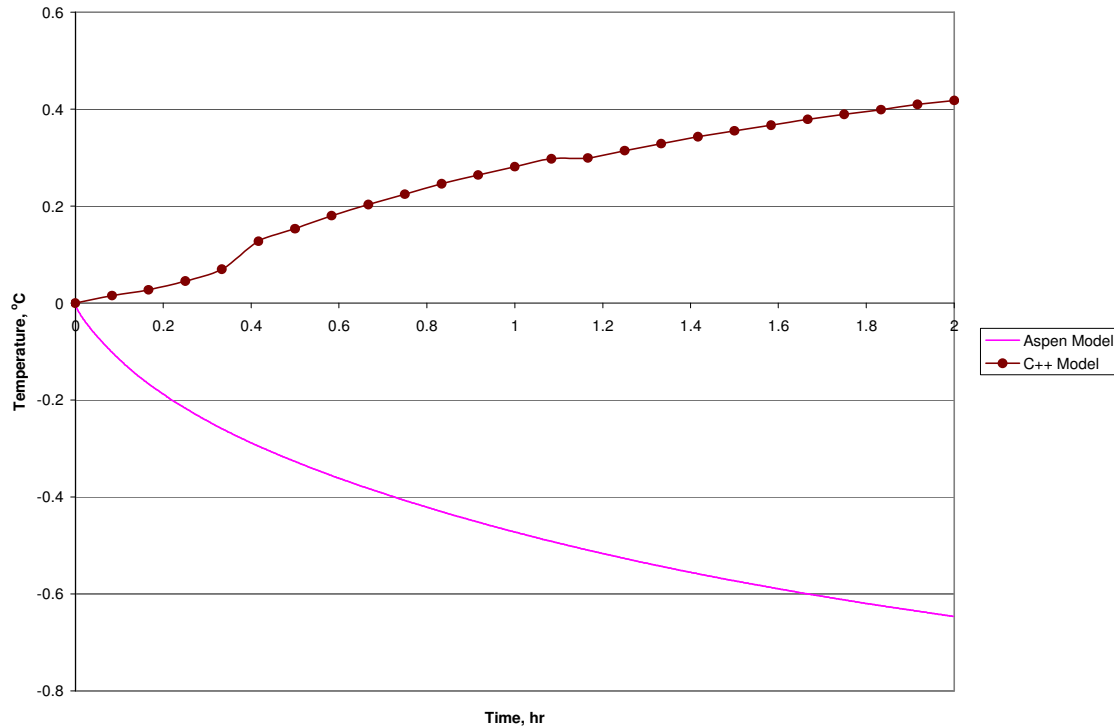

Figure 8.15 Response of dTA to a 5% change in Side Draw Flowrate

Figure 8.15 shows the effect that decreasing the side draw has on upper differential temperature measurement in the column. The side draw is the main product stream out of this column and represents approximately one third of the feed to the column. This plot shows that the temperatures react differently in each model to an increase in side product flowrate from the column. The Aspen model has problems converging with a large vapour side draw out of the column and thus the side draw in the Aspen model is taken as a liquid product. It should however be noted that the side draw from the actual column is a vapour side draw.

The results obtained from both models clearly do not match and once again this can be attributed to the distinctly different methods used in each model.

Plant data indicates that the effects of changes to side draw flow do not generally propagate to the top of the column. The upper differential temperature measurement is usually not very sensitive to this change because of the ratio controller on the actual plant that controls internal reflux to either side of the dividing wall below the chimney tray.
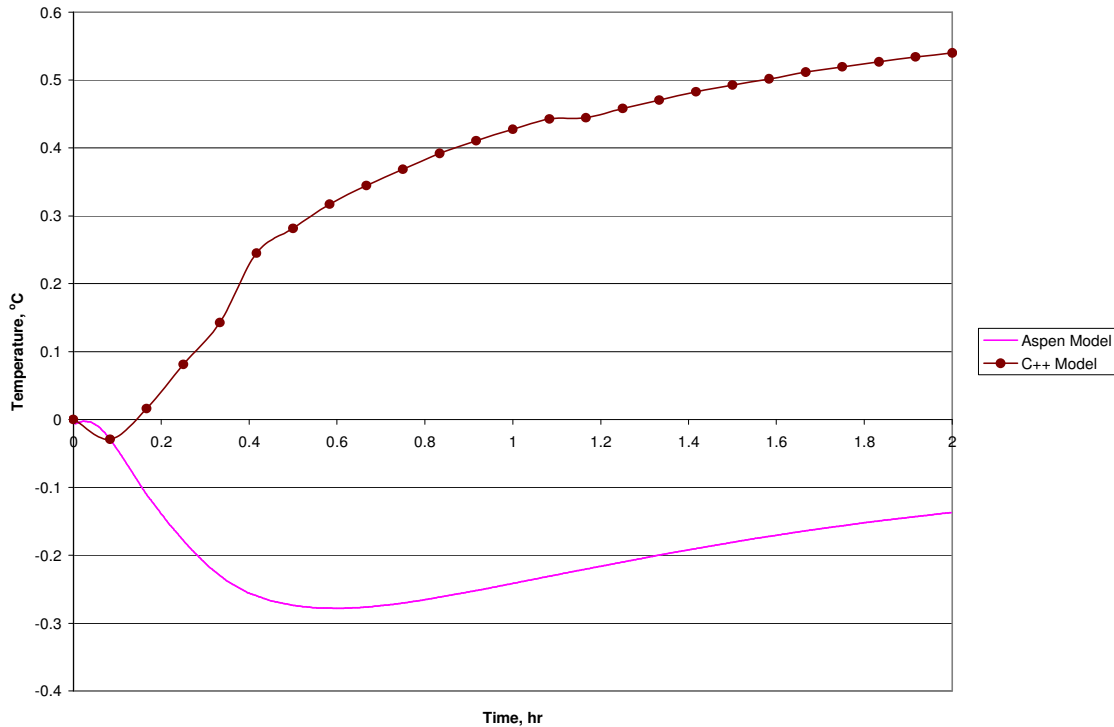

Figure 8.16 Response of dTB to a 5% change in Side Draw Flowrate

The effect that a decrease in side draw flowrate has on the lower differential temperature can be seen in figure 8.16. The Aspen and C++ models once again move in different directions.

The response of the Aspen model is similar to the response of a self regulating loop under PID control. The temperature overshoots and then slowly settles to a new steadystate. This is in keeping with the trends seen in the plant data. Figure 8.8 shows that dTB closely follows the side draw flowrate when it changes.

The above curves accurately represent the dynamics of each model developed. The results from the Aspen model is in keeping with trends seen from the 1-Octene plant data. The C+ model however does not match with the Aspen model or plant data. These response models were used to configure the multivariable controller. The controller was loaded with different

plant dynamics as gathered from testing each model. The code for this can be seen in Appendix A.

All the results from the step testing were in keeping with the trends that were expected based on the responses experienced on the actual plant as well as the Principles of Chemical Engineering.

It should be noted that the modelling techniques used in the C++ model is different to the techniques used by Aspentech in the simulation environment. Both models are, however comparable to the actual 1-Octene plant particularly at steadystate and have both been used for the control study. The curves in figures 8.8 to 8.15 show the differences in the dynamics of each model.

These empirical models were then used to configure the controller. The controller thus controls each model based on the dynamic information extracted from that particular model. Should there be the need to change any of the properties of the model, these step tests will need to be redone in order to configure the controller with the new models.

In industrial plants modifications are often made to the process for reasons of process optimisation or maintenance. These changes made to the plant affect the dynamics of that plant even though it may only be slight. It is for this reason that a lot of controllers tend to become ineffective after a while. Proper maintenance needs to be performed on multivariable controllers in order to keep them in good condition. The models in the controller should be periodically updated by doing new step testing when dynamics of the system change.

The DMC controller was used on the C++ and Aspen models for testing of the scheme that was created. The controller and C++ model were created in the same modelling environment. Testing of the model as well as testing of the controller was done using the same user interface as depicted in figure B2 in Appendix B.

The Aspen model could not be linked with the controller. The controller was thus run in step mode. The feedback of the control variables from the Aspen model were manually fed to the controller. The controller was then run for one execution cycle and the results for the manipulated variables were fed into the Aspen model. The Aspen model was then run for the same period of time and the process continued until sufficient data was collected.

We will first look at the results of the controller testing for the C++ Model. The feed flowrate was increased by 1 ton/hr which represents a feed disturbance of approximately 1.7 %.
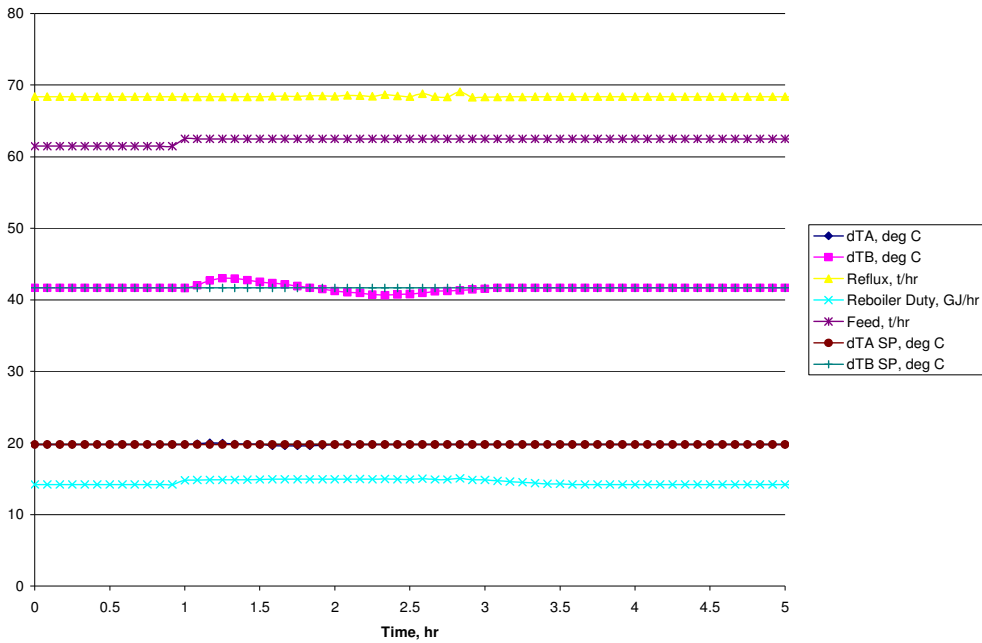

Figure 8.17 Controller test results for the C++ Model
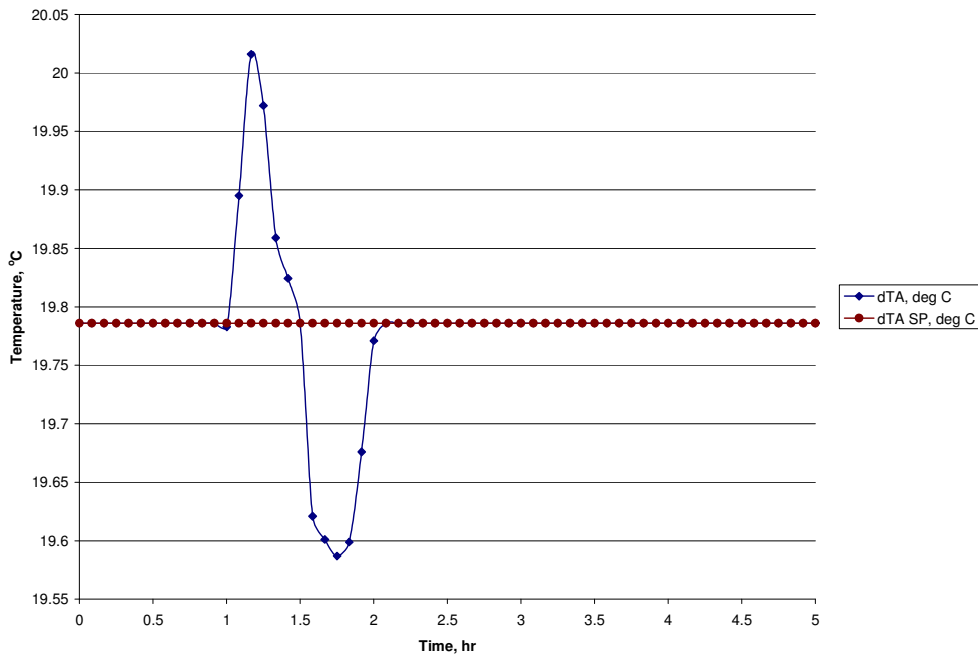

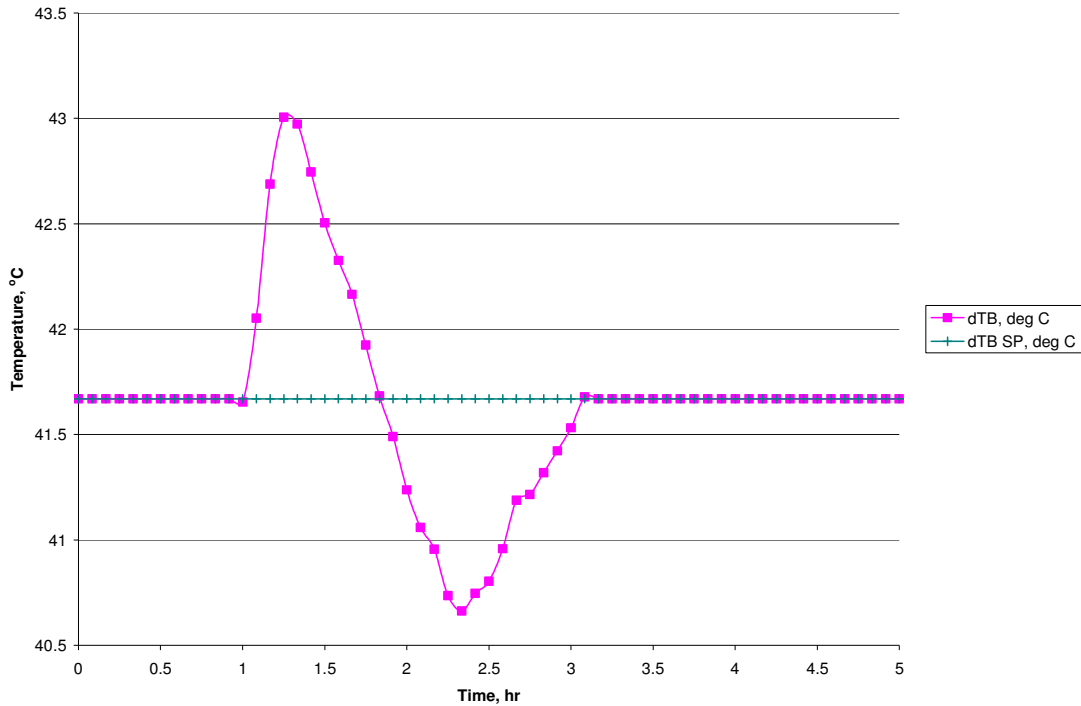Figure 8.18 Response of dTA to the controller test on the C++ Model

Figure 8.19 Response of dTB to the controller test on the C++ Model

The controller was tested by inducing an increase in feed flow to the column. The results in figures 8.17 to 8.19 clearly show that the controller is capable of rejecting disturbances that are introduced into the system.

The controller test carried out on the C++ model shows that the controller has been configured well on the model. Figures 8.17, 8.18 and 8.19 show that the controller works well on the C++ model even though the model does not match plant data. This is because the controller was set up based on the dynamics of the C++ model.

The controller is designed to control the process that it has been configured for irrespective of what the process is. The model does not give us a good indication with regards to the 1-Octene column performance. It does however show us that the controller works well.

The Aspen Controller was tested by also changing the feed flowrate to the column. Two decreases in feed flow of 0.5 tons/hr were induced on the system.
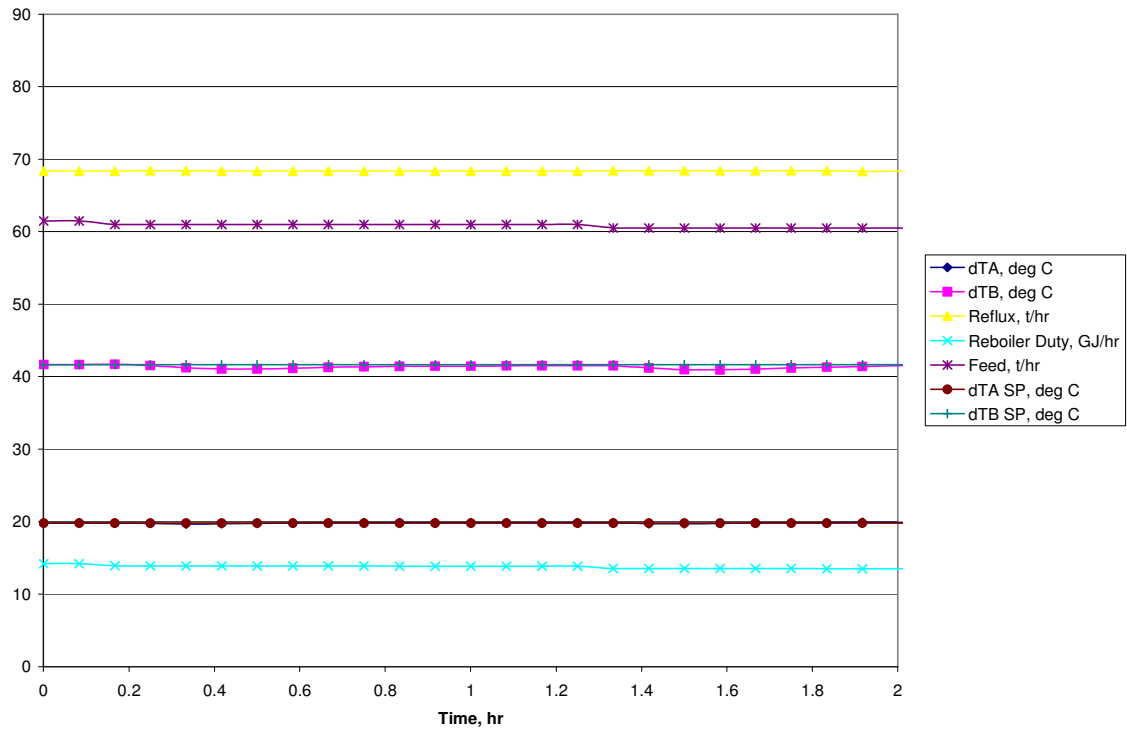
Figure 8.20 Controller test results for the Aspen Model
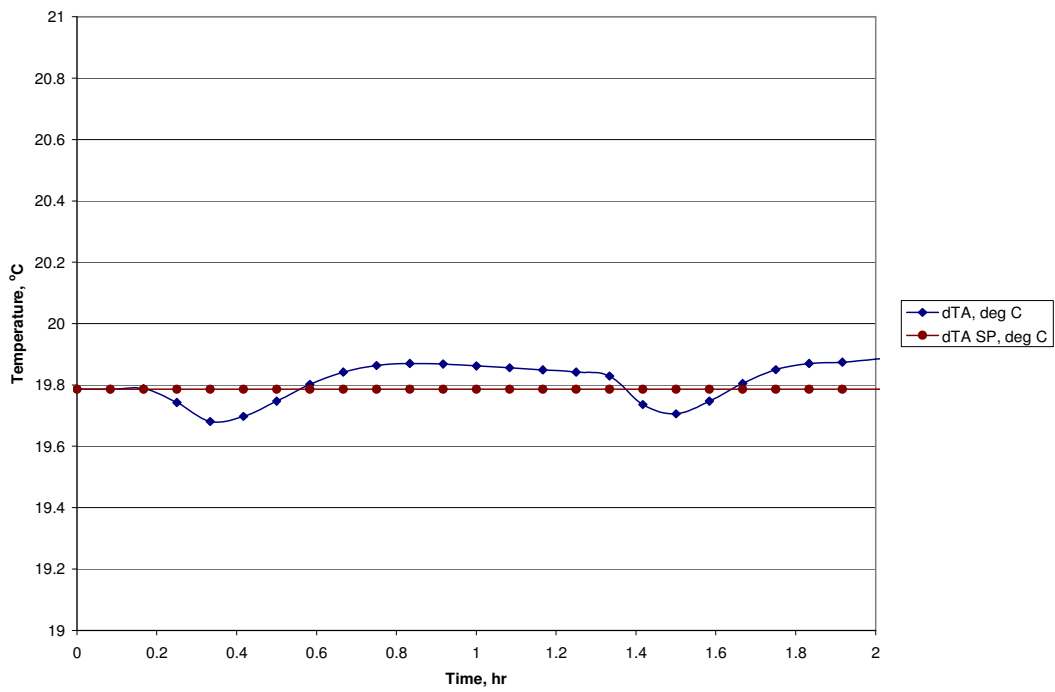

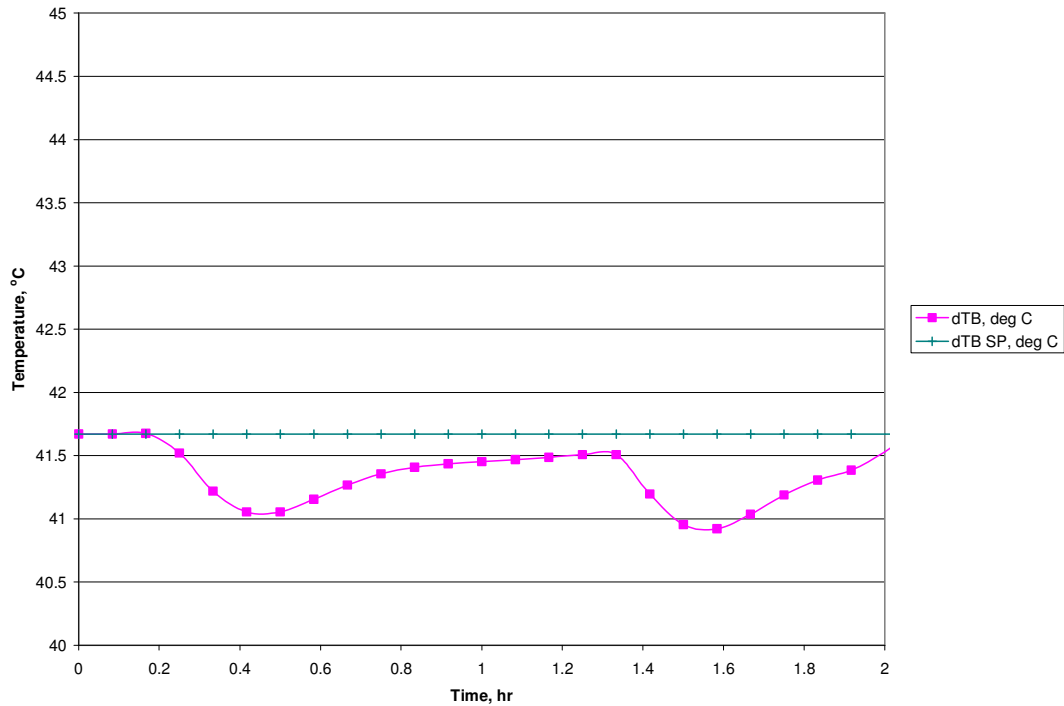Figure 8.21 Response of dTA to the controller test on the Aspen Model

Figure 8.22 Response of dTB to the controller test on the Aspen Model

The controller test on the Aspen model as depicted in figures 8.20, 8.21 and 8.22 also shows that the controller was capable of rejecting the disturbance that was introduced into the system.

Both models also show similarities in these tests. The increase in feed to the column increases the differential temperature measurements on the column in the C++ model. The decreases in feed temperature on the Aspen model showed the opposite effect.

During controller testing it was found that the controller is very aggressive in attempting to achieve its setpoints. This sometimes causes the controller to run into process constraints that have been imposed on the controller. A way in which this may be curbed is to set a range within which the controlled variables are to remain. This will help in creating a more robust multivariable controller.

Both models are more than suitable as representative models of the 1-Octene Plant. The controller has shown that it is capable of controlling the 1-Octene column. Advanced control should thus be seen as a solution to achieve stable operation on the 1-Octene column.

9. CONCLUSION

The chemical industry today faces a set of unique challenges that were not present previously. Emerging markets and competition has led to smaller profit margins while safety and environmental mandates require spending that reduces profit margins even further.

In order to be successful in the face of these challenges, plants must optimise production to take advantage of market opportunities, while minimising operating costs. The focus is thus aimed at plant reliability and availability which means that high variability, unit upsets, downtime, off-spec products are no longer acceptable.

Optimisation of operations and implementation of advanced control systems and smarter instrumentation is the direction that is being taken. The advanced controller developed is robust and capable of operating optimally and profitably.

Both models developed provided the required accuracy for this study at steady state. Two distinctly different methods of modelling a chemical plant were undertaken with the lumped parameter C++ not being representative of plant behaviour and the Aspen model was representative of plant behaviour.

Developing the lumped parameter model that was programmed in the C++ environment, enhanced understanding of all the phenomena that are occurring in the column. This type of modelling, however, is too complex if all phenomena are solved rigorously. Reasonably accurate short-cut methods were therefore used. These approximations prove to be good for steadystate modelling but not for dynamic modelling. The average temperatures calculated in each column section does not suffice. Rigorous modelling of every stage should be carried out as was done in the Aspen model.

A graphical user interface was created to facilitate easy manipulation of variables and to give a clearer view to the operation of the first principles model. The user interface created is similar to DCS graphics that operation staff uses. The column is graphically represented with all the controlled and manipulated variables visible on the same screen as well as all the advanced controller parameters and various different modes of operation. The same screen can be used when working with either model or plant feedback.

The Aspen model in contrast was developed by putting together the correct set of predefined functions. The fundamentals are the same and it allows greater detail to be included in the model. Rigorous equilibrium based calculation methods are used in order to increase the accuracy of the model developed. The dividing wall column is not a commonly used unit operation and thus a column of this nature is not part of the predefined unit operations. The dividing wall column can thus only be modelled by combining several standard unit operations.

The size of the controller designed was a 2x3 controller which does not include all of the column variables that affect the process. A bigger controller would have required more computing resources and would not have allowed enough time for all the investigations to be carried out in the time available. Should an industrial advanced controller be implemented on the column it should incorporate more variables. The side draw flowrate, internal reflux and other column temperature measurements would be included. Inferentials that are updated whenever lab sampling is done on the plant could also be included in the industrial advanced controller.

The use of an advanced controller maximises the recovery of 1-Octene by ensuring that the product is drawn at the correct temperature. Product losses to the overhead product is minimised by the upper differential temperature that is used by the controller.

The advanced controller also minimises the heat load to the column by manipulating the steam to the reboiler. Changes are only made by the controller in one minute intervals unlike in the case of having steam on PID control which aggressively reacts to every disturbance seen.

The 1-Octene column is a complex column to model, understand and operate due to its coupled nature. The operating range is constrained but the disturbances that the process experiences is mostly predictable from other measurements like feed rate. Based on the findings of this study the 1-Octene column is a strong candidate for implementation of industrial advanced control.

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APPENDIX A   DMC MICROSOFT VISUAL BASIC 6 PROGRAM CODE

The C++ solution of the DAE describing the system was performed using software developed by Professor Michael Mulholland.

Parts of the code used for the DMC Controller program is shown below:

```
// SET UP

  // PARAMETERS

  dtmax = 0.02;    // #### was 0.02
  pcmove_tol=10;   // max percentage move for any one variable before reevaluation of
                         Jacobians
  pertfr = 0.01;   // perturbation fraction
  minrespfr = 0.0*pertfr; // #### was 0.01, but should be 0.0 : minimum recognised
                         response fraction in "f" in perturbation evaluations
  minrange=1e-8;   // minimum allowed ranging for automatic Q & rR setting
  nexpm_max=1000;  // max number of iterations allowed for convergence in expm
                         calculation
  tol = 1e-3 ;     // Fractional Change Tolerance for matrix exponential convergence
  SM = 1e-8;       // Small value to protect against div-by-zero
  SMM = 1e-12;     // Smaller value for dvjj, g(equation sensitivity) and error report    SMMM =
1e-14;   // Smallest value for df, deriv & changemat
  SMtray = 10.0;   // Nominal minimum tray inventory [kmol]
  SMweedMt = 0;    // Smallest size element left in Mt sparse matrix (leaves 2 if -ve)
  SMweedCM = 0;        // Smallest size element left in CM sparse matrix (leaves 2 if -ve)
SMweedCMCI=0;    // Smallest size element left in CMCI sparse matrix (leaves 2 if -ve)
  SMc = 1e-7;      // Smallest upper constraint
  SMcf = 0.01;     // Minimum allowed constraint as factor of OBS
  BIG = 1e8;       // Maximum allowed gradient in Jacobian
  Matrix_Solution_TOLERANCE_fraction = 1e-3;   // for linear system solution in Step
Matrix_Solution_Shrink_Tol = 1e-8; // Absolute value for weeding intermediate matrix on
                                  each iteration
  Mt_START=0.01;       // Initialisation of Mt matrix : bigger value for slower change !
nFirstKrecalc = 1; // Number of initial recalculations of K (iterations) to get some convergence
  Kint = 10;       // No. of steps between re-evaluation of Kalman K
  Kcomp = 10;      // No. of compulsory initial re-evaluations of Kalman K
  QR100 =1;        // Q & rR scaling term #### was 1
  fast_response_factor=0.5;
  so_err_factor =  0.05;   // multiplies by relative "so" errors above to get observation
                               errors for observed variables only
  su_err_factor =  1.0// multiplies by relative "s" errors above to set unknown 'z' model
                    errors
```

```
f_err_factor  =  0.1;     // multiplies by relative "f" errors below to get equation errors
Rfactor       =  1;       // multiplies all elements of rR matrix
SlowReportLevel=0.80;     // slowdowns below this are reported
ncalls_until_reevaluation = 30; // after this many calls of execute, will force a
                                   reevaluation of all filter matrices
autoexpand=0.4;           // Automatic expansion of upper limits to max[SMcf*OBS,
                             shrink*(present value), (1+autoexpand)* (present value)]
                             on each step
shrink=0.95;              // factor for shrinking constraints #### was 0.95
MAX_av_obserr_pc = 5;     // av percent deviation from observations before reporting
MAX_av_deriverr_pc = 5;   // av percent imbalance in vessels based on largest inflow
LinSolnMethod = 3;        // Linear Solution:0=full MATLAB file; 1=sparse MATLAB file;
                             2=own sparse;  3=MATLAB Engine
FilterMethod = 3;         // Mt Update: 0=full MATLAB file; 1=using own full methods;
                             2=using own sparse methods;  3=using MATLAB Engine;
REINITIALISE_Mt_FOR_NEW_OBSMODE = 1;   // 1 = don't just continue using old
                                          Mt, restart with small diagonal
speedupfactor = 1.0;      // #### WARNING, THIS SHOULD BE 1.0 FOR NORMAL
                             REAL-TIME OPERATION !
```

Initialisation:

```
AUTOdmc=0;                // auto/manual switch
Ndmc=24;                  // horizon : 24 * 5min = 2hours
Mdmc=1;                   // optimised moves
Pdmc=2;                   // manipulated variables
Qdmc=1;                   // disturbance variables
Rdmc=2;                   // controlled variables
eol.Init(Ndmc*Rdmc,1);
B.Init(Ndmc*Rdmc,Mdmc*Pdmc);
Bol.Init(Ndmc*Rdmc,Ndmc*(Pdmc+Qdmc));
B0.Init(Ndmc*Rdmc,Ndmc*(Pdmc+Qdmc));
Bol_B0.Init(Ndmc*Rdmc,Ndmc*(Pdmc+Qdmc));
dmp.Init(Ndmc*(Pdmc+Qdmc),1);
dm.Init(Mdmc*Pdmc,1);
dml.Init(Pdmc+Qdmc,1);
Wdmc.Init(Ndmc*Rdmc,Ndmc*Rdmc);
Ldmc.Init(Mdmc*Pdmc,Mdmc*Pdmc);
Kdmc.Init(Mdmc*Pdmc,Ndmc*Rdmc);
x0.Init(Ndmc*Rdmc,1);
xsp.Init(Ndmc*Rdmc,1);
graderr.Init(Ndmc*Rdmc,1);
lasterr.Init(Ndmc*Rdmc,1);
trajerr.Init(Ndmc*Rdmc,1);
mlast.Init((Pdmc+Qdmc),1);
resp.Init(Ndmc,Rdmc*(Pdmc+Qdmc+1)); // just for loading the responses
```

Configuring the Controller matrix with step test data:
resp(1,1) =0.09;   resp(1,2) =0.11;   resp(1,3) =-0.25;   resp(1,4) =-0.05;
resp(1,5) =-0.02;   resp(1,6) =-0.09;   resp(1,7) =-0.08;   resp(1,8) =-0.04;

resp(2,1) =   0.17; resp(2,2) =0.18;   resp(2,3) =-0.37;   resp(2,4) =-0.12;
resp(2,5) =-0.06;   resp(2,6) =-0.13;   resp(2,7) =-0.10;   resp(2,8) =-0.01;
.   .   .   .
.   .   .   .
.   .   .   .
.   .   .   .
.   .   .   .
.   .   .   .
.   .   .   .
resp(22,1) =0.13;   resp(22,2) =0.44;   resp(22,3) =-6.65;   resp(22,4) =-6.40;
resp(22,5) =0.35;   resp(22,6) =0.47;   resp(22,7) =-0.09;   resp(22,8) =0.13;

resp(23,1) =0.13;   resp(23,2) =0.45;   resp(23,3) =-6.64;   resp(23,4) =-6.39;
resp(23,5) =0.36;   resp(23,6) =0.48;   resp(23,7) =-0.10;   resp(23,8) =0.12;

resp(24,1) =0.13;   resp(24,2) =0.47;   resp(24,3) =-6.62;   resp(24,4) =-6.38;
resp(24;5) =0.37;   resp(24,6) =0.50;   resp(24,7) =-0.10;   resp(24,8) =0.12;

Model mod;   // Create the Model

  // Initialisation Options
mod.CONSTRAINTSFROMLAST=1;   // Base constraints on the State at the end of the
                                  last run
mod.STARTATLAST=1;   // Start state values at their values at the end of the
                                  last run
mod.LOADLASTMT=1;   // Load Kalman Filter Covariance matrix from end
                                  of last run instead of re-initialising

  mod.Initialise();

// **Any observations or time-changes---**

        // R=1 => recognise observation
        //
        // ....SMFio(el) = SMFdat;   SMFioR(el) = 0/1;
        // =====So(el) = Ldat;   SoR(el) = 0/1;
   double FeedMassFlow = 61.476;   // [t / h]
      mod.Ratefeed = FeedMassFlow*1000/mod.MMF; // [kmol/h]

//Tray Volumes (per single tray in each section type):

```
    //(Reboiler & accumulator have a larger volumes)
    cMatrix<double> Vtray;
    Vtray.Init((mod.NS+mod.NP),1);
    Vtray(1) = 4.0; // Condenser / Accumulator [m3
    Vtray(2) = 8.856*0.0652 ; // A Top   [m3]
    Vtray(3) = 5.856*0.0594 ; // B Feed  [m3]
    Vtray(4) = 5.856*0.0575 ; // C Feed  [m3]
    Vtray(5) = 12.167*0.064 ; // D Bottom  [m3]
    Vtray(6) = 3.0 ; // Reboiler  [m3
    Vtray(7) = 5.856*0.0681 ; // B Draw  [m3]
    Vtray(8) = 5.856*0.0569 ; // C Draw  [m3]
    Vtray(9) = 0.3*Vtray(2) ; // Feed Flash [m3] (dummy)  ... must be small - not real

    for (i=1;i<=(mod.NS+mod.NP); i++)
    {
       mod.Mo(i) = mod.NT(i)*Vtray(i)*DensAv;  // [kmol] based on average density
       mod.MoR(i)= 1;
    }
```

// Average Pressure in each section

```
    double PtopSet = 1.85; //####1.85;  // [bara]
    mod.P(1) = PtopSet;
    mod.P(2) = PtopSet+0.5*mod.NT(2)*0.0652*mod.MMF*DensAv*9.81/1e5;
    mod.P(3)              =              PtopSet+(0.5*mod.NT(3)*0.0594              +
    mod.NT(2)*0.0652)*mod.MMF*DensAv*9.81/1e5;
    mod.P(4)     =     PtopSet+(0.5*mod.NT(4)*0.0575     +     mod.NT(3)*0.0594     +
    mod.NT(2)*0.0652)*mod.MMF*DensAv*9.81/1e5;
    mod.P(5) = PtopSet+(0.5*mod.NT(5)*0.0640 + mod.NT(4)*0.0575 + mod.NT(3)*0.0594 +
    mod.NT(2)*0.0652)*mod.MMF*DensAv*9.81/1e5;
    mod.P(6) = PtopSet+((1+mod.NT(5))*0.0640 + mod.NT(4)*0.0575 + mod.NT(3)*0.0594 +
    mod.NT(2)*0.0652)*mod.MMF*DensAv*9.81/1e5;
    mod.P(7)              =              PtopSet+(0.5*mod.NT(7)*0.0681              +
    mod.NT(2)*0.0652)*mod.MMF*DensAv*9.81/1e5;
    mod.P(8)     =     PtopSet+(0.5*mod.NT(8)*0.0569     +     mod.NT(7)*0.0681     +
    mod.NT(2)*0.0652)*mod.MMF*DensAv*9.81/1e5;
    mod.P(9) = mod.Pfeed;
```

APPENDIX B   GRAPHICS
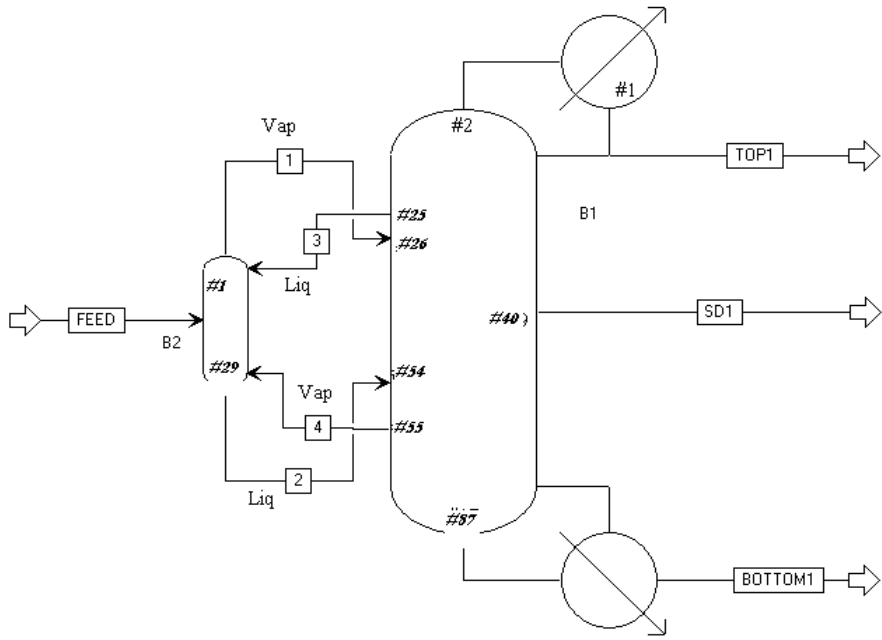

Figure B1   Representation of the dividing wall column in Aspen Plus
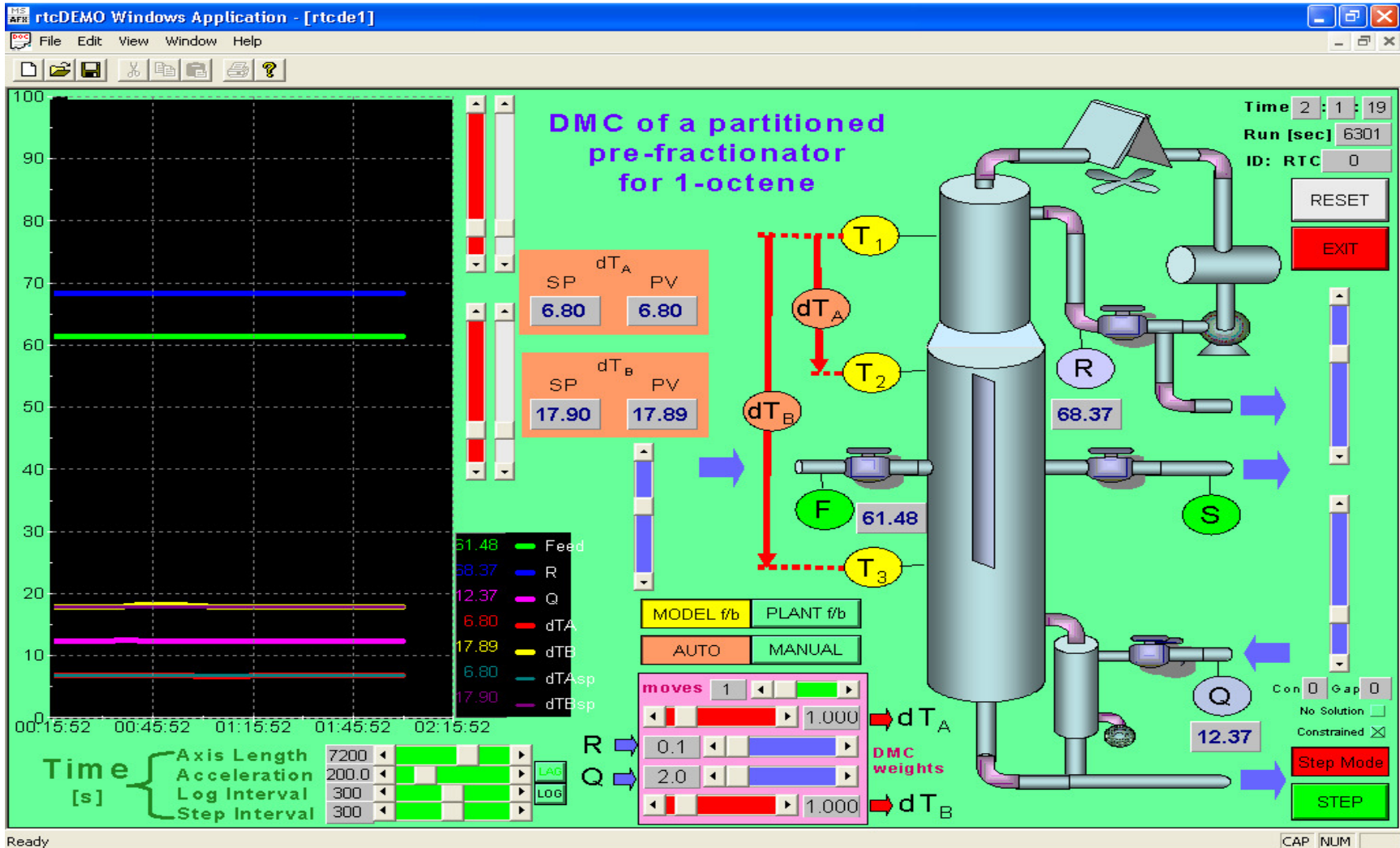
Figure B2   Graphical faceplate used for C++ Model
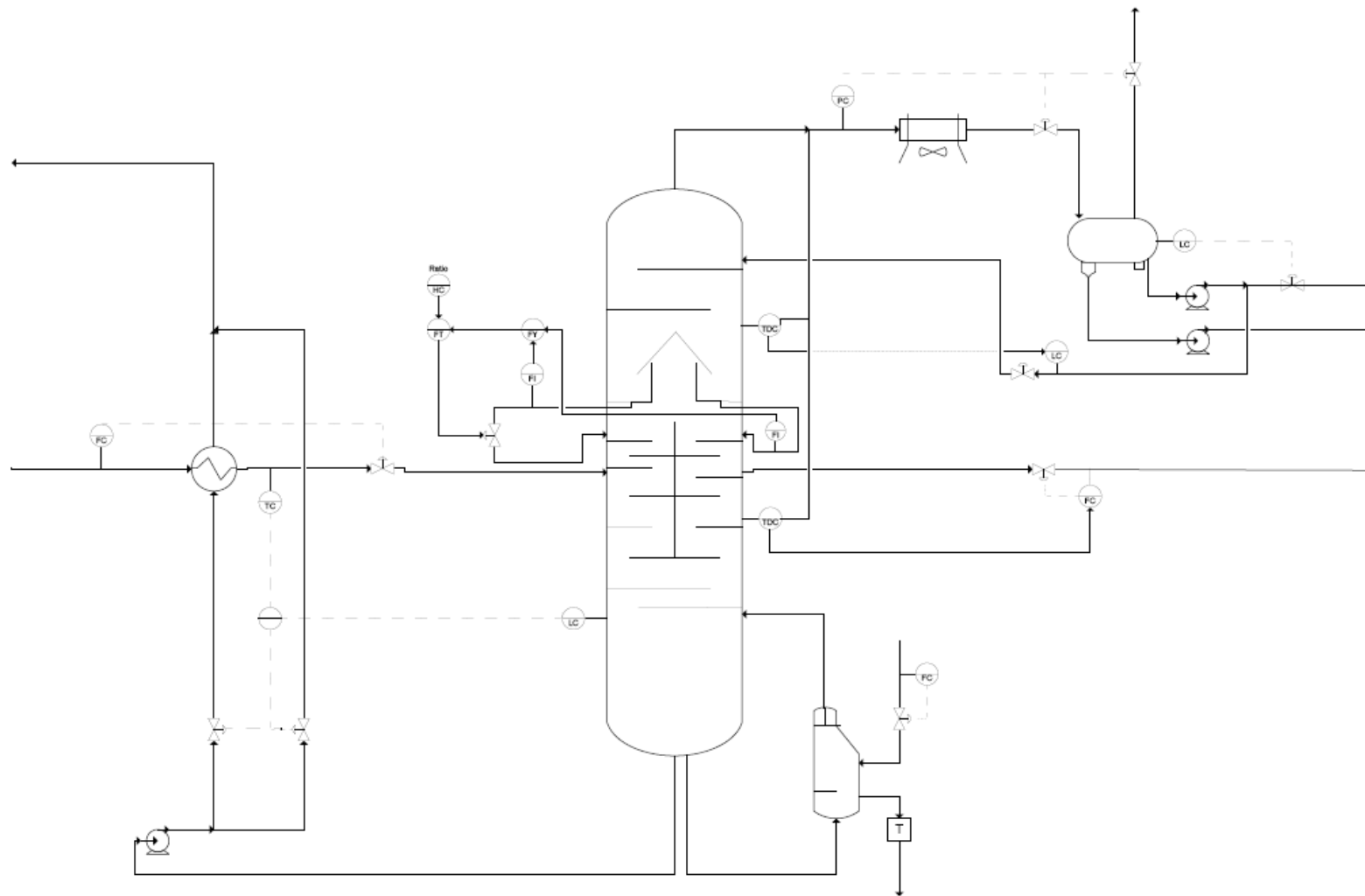
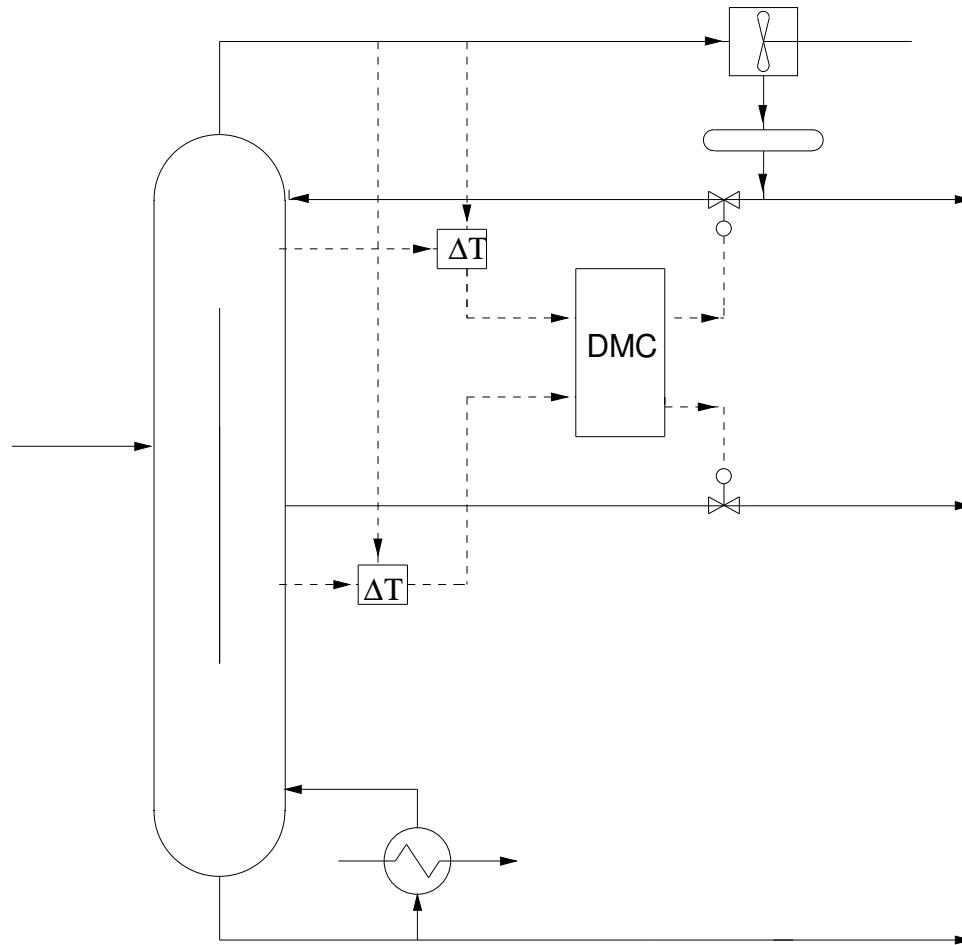Figure B3   Simplified P&ID of the 1-Octene Column

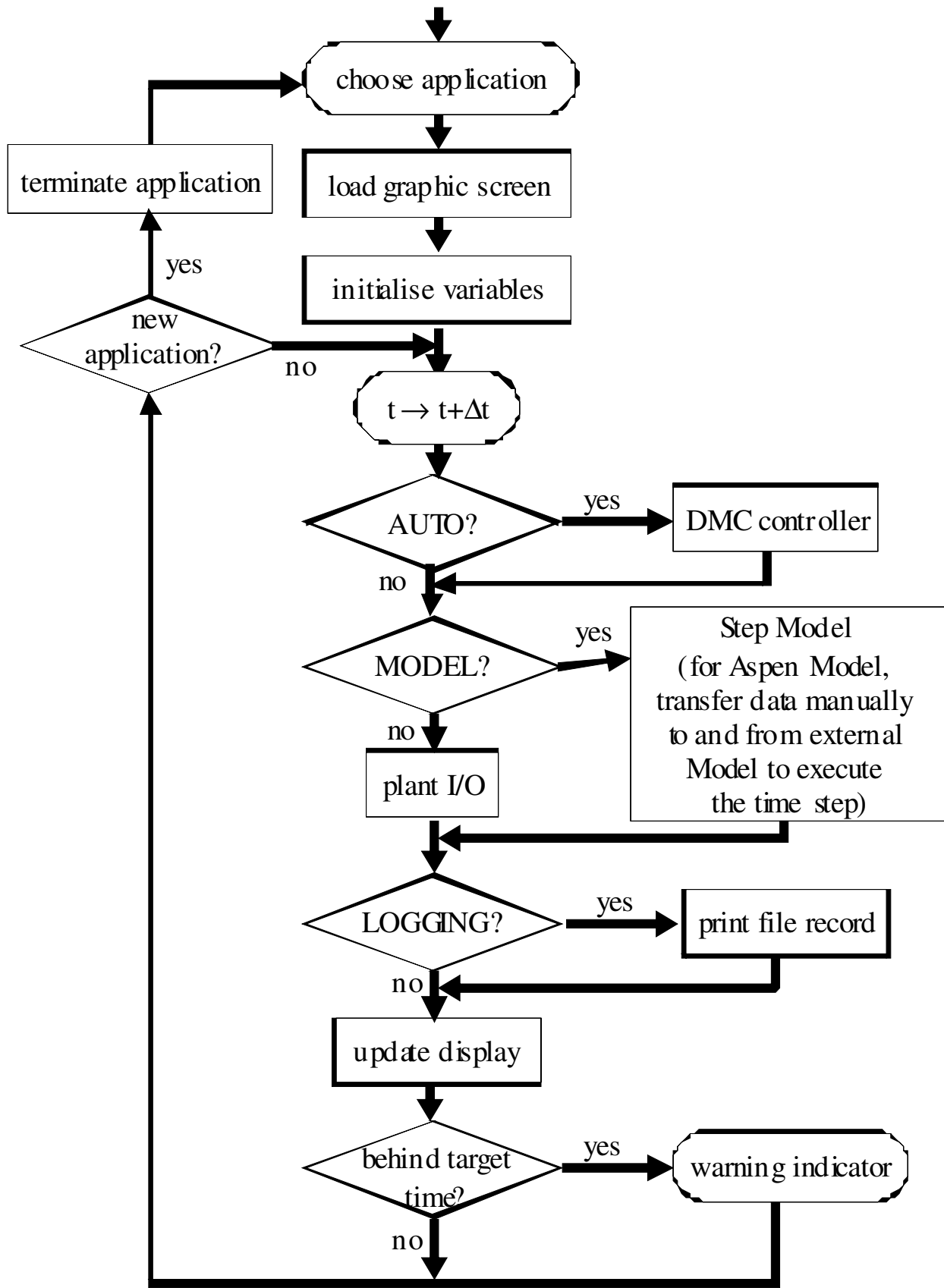Figure B4   Simplified P&ID of the 1-Octene Column Advanced Control Strategy

Figure B5   Block Diagram of the Execution Cycle for C++ Model Class