

**INTEGRATED PRODUCTION FOR  
OIL REFINERIES AND PETROCHEMICAL PLANTS**

A thesis submitted to The University of Manchester for the degree of

**Doctor of Philosophy**

in the Faculty of Engineering and Physical Sciences

**2005**

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## **List of Contents**

List of Contents.....	2
List of Figures.....	6
List of Tables.....	10
Abstract.....	11
Declaration .....	13
Copyright Statement.....	14
Acknowledgements.....	15
List of Abbreviations.....	16
<b>Chapter 1 Introduction.....</b>	<b>18</b>
1.1 Production Planning Problem.....	19
1.2 Analysis and Optimisation of Integrated Production Planning.....	25
1.3 Problem Statement, Aim and Objectives.....	28
1.4 Synopsis.....	29
1.5 References.....	30
<b>Chapter 2 Literature Review.....</b>	<b>31</b>
2.1 Review of Production Planning Problem.....	32
2.2 Flexibility of Production Planning.....	33
2.3 Integrated Production Planning.....	35
2.4 Gaps in Previous Works.....	37
2.5 References.....	38

<b>Chapter 3 Modelling Strategy</b> .....	42
3.1 Introduction.....	43
3.2 Site Level Modelling.....	46
3.2.1 Mixer Model.....	49
3.2.2 Splitter Model.....	50
3.3 Process Level Modelling.....	50
3.3.1 Crude Distillation Model.....	51
3.3.2 Hydrotreaters Model.....	52
3.3.3 Catalytic Reformer Model.....	53
3.3.4 Fluid Catalytic Cracker Model.....	55
3.3.5 Aromatic Production Model.....	57
3.3.6 Steam Cracker Model.....	59
3.3.6.1 Development of Steam Cracker Model.....	59
3.4 Overall Formulation.....	65
3.5 Summary.....	67
3.6 References.....	68
<b>Chapter 4 Planning for Integrated Production of Oil Refinery and Petrochemical Plant</b> .....	70
4.1 Introduction.....	71
4.2 Hierarchy of Production Planning Process.....	71
4.3 Production Planning Models.....	73
4.4 Features of Integrated Production Planning.....	77

4.4.1 Modelling Integrated Production.....	79
4.5 Case Study: Integrated oil refinery and petrochemical production for profit maximisation.....	81
4.6 Summary.....	90
4.7 References.....	91
<b>Chapter 5 Strategies for Implementation of Integrated Production...</b>	93
5.1 Implementation Issues.....	94
5.2 Analysis of Necessity for Integrated Production.....	95
5.2.1 Supply-Demand Pricing Model.....	96
5.2.2 Cost-Plus Pricing Model.....	98
5.2.3 Determining the Price of Exchanging Materials.....	100
5.2.4 Determining the Necessity for Integrated Production.....	104
5.3 Computational Difficulty.....	106
5.3.1 Sequential Optimisation Approach.....	108
5.4 Difficulty of Sharing Proprietary Process Models.....	110
5.5 Case Study 2: Application of New Strategies to Implement Integrated Production.....	115
5.6 Summary.....	120
5.7 References.....	121
<b>Chapter 6 Uncertainty and Flexibility.....</b>	122
6.1 Introduction.....	123
6.2 Uncertainty in Demand and Prices.....	124

6.3 Quantifying Uncertainty.....	126
6.3.1 An Example for Quantifying Uncertainty.....	129
6.4 Solution Approaches to Problems with Uncertainty.....	131
6.4.1 An Example of Production Planning under Uncertainty.....	133
6.5 Feasibility Analysis of Integrated Production Planning under Uncertainty...	134
6.6 Case Study 3: Flexible Integrated Production under Uncertain Demand and Prices.....	137
6.7 Summary.....	145
6.8 References.....	146
<b>Chapter 7 Conclusions and Future Work.....</b>	<b>147</b>
7.1 Conclusions and Significance.....	148
7.2 Future Work.....	151
<b>Appendix A Cost Data .....</b>	<b>153</b>
<b>Appendix B Yield Correlations for Refinery and     Petrochemical Process Units.....</b>	<b>156</b>
B1. Crude Distillation Unit.....	157
B2. Aromatics Production Unit.....	158
B3. Steam Cracker Production Unit.....	160

## **List of Figures**

### **Chapter 1 Introduction**

Figure 1.1: Fuel production supply-chain.....	20
Figure 1.2: Petrochemical production supply-chain.....	20
Figure 1.3: Price differentials analysis against crude oil price.....	21
Figure 1.4: A 60-month naphtha price trend.....	22
Figure 1.5: Price differentials analysis against natural gas price.....	23
Figure 1.6: Decision making in production planning problem.....	23
Figure 1.7: Integration of final products.....	26
Figure 1.8: Integration of intermediate products.....	27
Figure 1.9: Integration of processing unit.....	27

### **Chapter 3 Modelling Strategy**

Figure 3.1: An oil refinery flowsheet incorporating an aromatic production unit..	44
Figure 3.2: General outline of a petrochemical plant complex.....	45
Figure 3.3: A petrochemical plant flowsheet for the production of basic chemicals.....	46
Figure 3.4: A generalized plant configuration.....	47
Figure 3.5: Unit operating cost as a function of process unit throughput.....	48
Figure 3.6: TBP curves for Heavy (Arabian Heavy) and Light (Brent) crudes...	52
Figure 3.7: Reformate yield as a function of <b>N2A</b> .....	54
Figure 3.8: Reformate yield as a function of <b>RON</b> .....	54

Figure 3.9: Effect of FCC conversion on gasoline and coke yields.....	56
Figure 3.10: Gasoline RON as a function of yield.....	56
Figure 3.11: Effect of reformate quality on BTX yield.....	58
Figure 3.12: Comparison of BTX yields from reformate and pygas.....	59
Figure 3.13: Correlations between density of alkanes and $\chi^T$ .....	60
Figure 3.14: Correlations between boiling points of alkanes and $\chi^T$ .....	61
Figure 3.15: Parity plot for ethane-propane correlation model.....	63
Figure 3.16: Parity plot for naphtha correlation model.....	63
Figure 3.17: Model prediction for the steam-cracking of 80/20 ethane-propane feed at varying temperature and fixed residence time of 0.35 s.....	64
Figure 3.18: Model prediction for the steam-cracking of heavy naphtha feed at varying temperature and residence time of 0.35 s.....	64

**Chapter 4 Planning for Integrated Production of  
Oil Refinery and Petrochemical Plant**

Figure 4.1: Hierarchy in the planning of process plant production.....	73
Figure 4.2: Interaction of LP model with a simulation model.....	75
Figure 4.3: Demand constraints for oil refinery production.....	83
Figure 4.4: Demand constraints for petrochemical plant production.....	83
Figure 4.5: Petrochemical's naphtha feed selection during stand-alone and integrated production.....	84
Figure 4.6: Petrochemical's gasoil feed selection during stand-alone and integrated production.....	85
Figure 4.7: Comparison of optimum crude oil mix between stand-alone and integrated production strategies.....	85

Figure 4.8: Feed source for the production of xylene during stand-alone and integrated production.....	86
Figure 4.9: Comparison of major product distributions during stand-alone and integrated production.....	87
Figure 4.10: Process connectivity between oil refinery and petrochemical plant in a multi-period integrated production plan.....	88
Figure 4.11: Comparison of FCC coking profile during stand-alone and integrated production strategies.....	90

### ***Chapter 5 Strategies for Implementation of Integrated Production***

Figure 5.1: Supply-demand pricing model.....	96
Figure 5.2: A typical cost-plus pricing model to determine PPP.....	100
Figure 5.3: Effect of naphtha price change on the change of netback for oil refinery and petrochemical plant.....	104
Figure 5.4: Sequential optimisation approach.....	110
Figure 5.5: Interaction model.....	111
Figure 5.6: Generalized implementation procedures.....	114

### ***Chapter 6 Uncertainty and Flexibility***

Figure 6.1: Historical profile of uncertainty in naphtha demand and price.....	125
Figure 6.2: Historical profile of uncertainty in gasoil demand and price.....	125
Figure 6.3: Quantifying naphtha price uncertainty.....	127
Figure 6.4: Quantifying naphtha demand uncertainty.....	128
Figure 6.5: Cumulative distribution function for Example 6.3.1.....	130



Figure 6.6: Approaches to the analysis of a flexible integrated production plan...	136
Figure 6.7: Comparison of crude oil feed profiles between normal production planning and planning under uncertainty.....	138
Figure 6.8: Comparison of naphtha feed profile between normal production and planning under uncertainty.....	139
Figure 6.9: Comparison of gasoil feed profile between normal production and planning under uncertainty.....	139
Figure 6.10: Propylene integration during normal production planning and planning under uncertainty.....	140
Figure 6.11: Comparison of integrated production during normal planning and during planning under uncertainty.....	141
Figure 6.12: Infeasible production of gasoline 95# during planning under uncertainty.....	142
Figure 6.13: Feasible production of gasoline 95# during planning under uncertainty with relaxed demand constraint.....	143
Figure 6.14: Feasible production of gasoline 95# during planning under uncertainty with increased starting inventory during period 1.....	143

## **List of Tables**

### **Chapter 4 Planning for Integrated Production of Oil Refinery and Petrochemical Plant**

Table 4.1: An example of MPS.....	72
Table 4.2: Major constraints for oil refinery and petrochemical plant operations.....	82

### **Chapter 5 Strategies for Implementation of Integrated Production**

Table 5.1: Calculation of naphtha's plant posted price (PPP) .....	101
Table 5.2: Calculation of refinery and petrochemical netback.....	103
Table 5.3: Sensitivity analysis to determine the necessity for integration.....	105
Table 5.4: Sensitivity analysis to determine the necessity for propylene integration.....	117
Table 5.5: Comparison of performance between simultaneous and sequential optimisation approach.....	118

### **Chapter 6 Uncertainty and Flexibility**

Table 6.1. A 12-period historical demand of gasoil.....	129
Table 6.2. Frequency of demand occurrence within $\pm 3\sigma$ .....	129
Table 6.3. Probability function for the demand of a refinery product.....	130
Table 6.4. Data for uncertainty in naphtha demand and prices.....	137
Table 6.5: Comparison of performance between normal production planning and planning under uncertainty.....	144

## ***Abstract***

In an increasingly globalised commodity market and under continually changing economic scenarios, oil, gas and petrochemical plants are forced to improve their operation practices in order to remain competitive. One strategy that can be adopted is to exploit the synergy between oil refineries and petrochemical plants through the strategy of integrated production. In this work, issues of integrated production strategy with respect to profitability, implementation and flexibility are explored. Profitability is the key motivation for any plant to change its operation practices. Three options for the strategy of integrated production are considered: integration of final products, integration of intermediate products, and integration of processing units. Decisions are made on the allocation of material resources, the distribution of products and the operating conditions of process units. These decisions are optimised for maximum profit while satisfying all production constraints. In the integrated production of an oil refinery and a petrochemical plant, propylene, naphtha, gasoil and pygas are selected for integration. The benefits of the integrated production strategy are lower costs and higher profits to the integrated plants. Systematic implementation of integrated production strategy is carried out by evaluating the necessary condition and generating an interaction model to bridge information flow between the two plants. Sensitivity analysis is used to evaluate the necessary condition for integrated production. The interaction model regulates the required information flow between the two plants and screens for options of integrated production network. Flexibility of integrated production plan is studied by varying demands and prices of exchanged materials. For an integrated production plant to be

flexible, it has to remain feasible even when these parameters change. Flexibility analysis allows steps to be carried out at an early stage to ensure feasibility of the integrated production plan. All integrated production planning problems are formulated as non-linear programming problem (NLP) and solved using the modular sequential optimisation approach. Case studies are performed to demonstrate how the three issues are addressed.

### ***Declaration***

No portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institution of learning.

Shuhaimi Mahadzir

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## ***Acknowledgements***

I would like to express my deep gratitude to my supervisor, Dr Nan Zhang, for his guidance and support throughout my research and study. I have found no words to describe my sincere appreciation on the countless discussions we have had leading to the completion of this thesis.

My appreciation goes to UTP for supporting me financially to study at UMIST and later known as The University of Manchester.

Special thanks to the Centre for Process Integration for giving me the opportunity to gain the benefit of studying in a truly international environment. My appreciations go to the staffs and fellow students at the Centre for Process Integration for their friendship and help in every way through out the duration of my study.

Sincere and unbounded thanks to my parents, my wife and my children for all their love and prayers. I look forward to be with all of you again back home.

## List of Abbreviations

<b><i>c</i></b>	unit cost or price
<b><i>f</i></b>	general function
<b><i>n</i></b>	number of data points
<b><i>x</i></b>	plant yields
<b><i>y</i></b>	general variables
<b><math>\bar{y}</math></b>	average of <b><i>y</i></b>
<b><i>AP</i></b>	aniline point
<b><i>CI</i></b>	total inventory cost
<b><i>CM</i></b>	total material cost
<b><i>CP</i></b>	total production cost
<b><i>CT</i></b>	total cost plant
<b><i>D</i></b>	demand
<b><i>F</i></b>	flow rate
<b><i>FQP</i></b>	feed quality parameter
<b><i>I<sub>M</sub></i></b>	molecular index
<b><i>I<sub>S</sub></i></b>	severity index
<b><i>N2A</i></b>	naphthene plus 2 times aromatics
<b><i>P</i></b>	pressure
<b><i>p(y)</i></b>	probability function of <b><i>y</i></b>
<b><i>PPP</i></b>	plant posted price
<b><i>Pr</i></b>	probability
<b><i>PR</i></b>	profit rate
<b><i>Q</i></b>	plant capacity
<b><i>QI</i></b>	inventory holding
<b><i>RON</i></b>	research octane number
<b><i>RT</i></b>	total revenue
<b><i>S</i></b>	sulphur content
<b><i>SG</i></b>	specific gravity
<b><i>VABP</i></b>	average boiling point

## Indices

<b><i>i</i></b>	inlet flow
<b><i>j</i></b>	outlet flow
<b><i>n</i></b>	process unit



*p* process plant  
*s* scenarios  
*t* period

### **Subscripts**

*D* demand  
*F* fixed  
*G* general  
*I* inventory  
*OP* operating  
*S* supply  
*V* variable

### **Superscripts**

*E* enterprise  
*L* lower limit  
*U* upper limit

### **Greeks**

$\alpha$  multiplier for stream allocation  
 $\beta$  confidence level  
 $\gamma$  physical properties  
 $\zeta$  chemical compositions  
 $\theta$  residence time  
 $\kappa$  Arrhenius constant  
 $\lambda$  rate of supply/demand change  
 $\sigma$  standard deviation  
 $\varsigma$  penalty charge  
 $\varphi$  operating conditions  
 $\chi$  Randic's index  
 $\Xi$  quantity demand/supply  
 $\Pi$  price  
 $\Phi$  cumulative distribution function

## ***Chapter 1 Introduction***

1.1 Production Planning Problem.....	19
1.2 Analysis and Optimisation of Integrated Production Planning.....	25
1.3 Problem Statement, Aim and Objectives.....	28
1.4 Synopsis.....	29
1.5 References.....	30

## ***1.1 Production Planning Problem***

In today's globalised economy, efficient usage of available production resources becomes increasingly important to industry. Economic globalisation and market liberalisation have forced many companies in the oil and petrochemical industries to re-evaluate and improve the way in which they run and manage their plants. Globalisation has also created a situation where plants have seen shortages of feed materials and rising prices due to strong demands (Shell, 2005).

Fuel and petrochemical supply chains are also becoming more overlapping. For example, naphtha can either be upgraded into gasoline or cracked for the manufacture of ethylene. In addition, the advent of gas-to-liquid technology has seen natural gas – a primary feed material for the petrochemical industry – becoming a commodity for middle distillate fuel production. Figures 1.1 and 1.2 illustrate the overlapping phenomena of the hydrocarbon supply chain in the petroleum fuel and petrochemical industries.

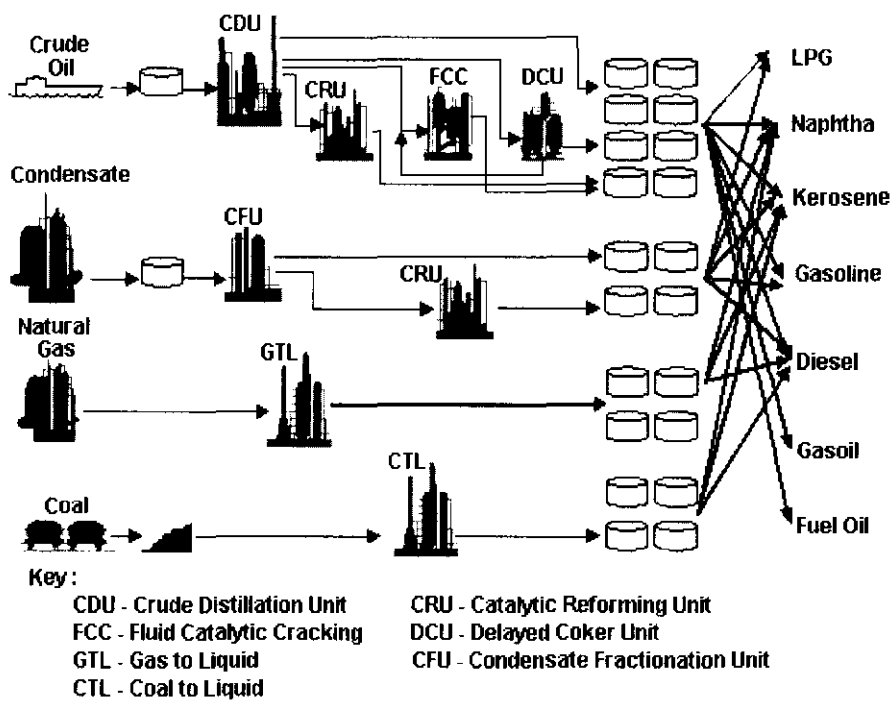


Figure 1.1: Fuel production supply-chain

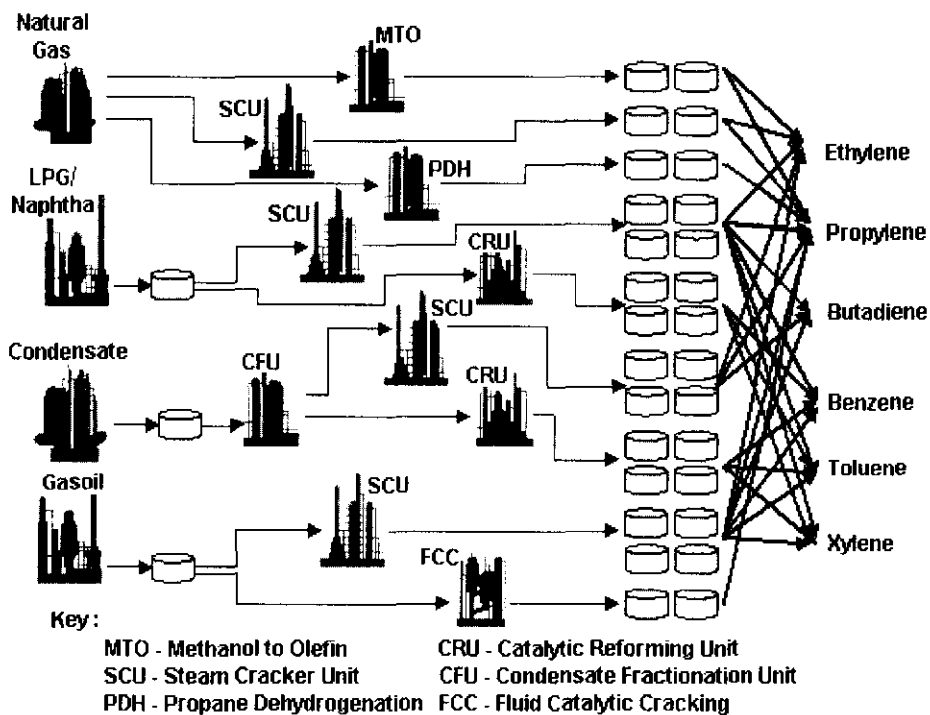
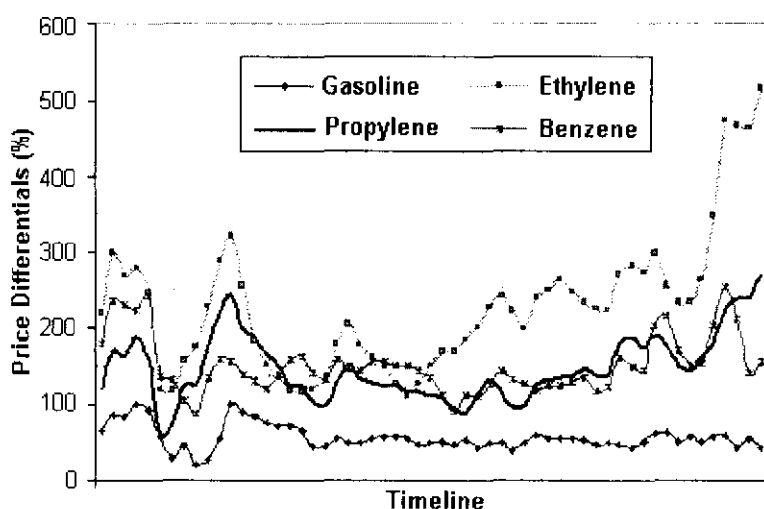


Figure 1.2: Petrochemical production supply-chain

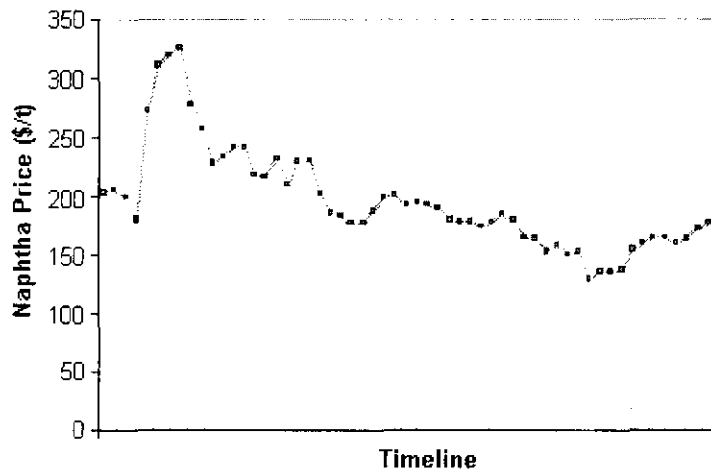
The reasons why fuel and petrochemical industries often compete for the same hydrocarbon resources can perhaps be understood by performing price differentials analysis. Price differentials are calculated as the relative differences between the prices of products and the prices of feeds. Figure 1.3 shows the trend of historical price differentials for petroleum fuel, olefin and aromatic products against the historical price



**Figure 1.3: Price differentials analysis against crude oil price**

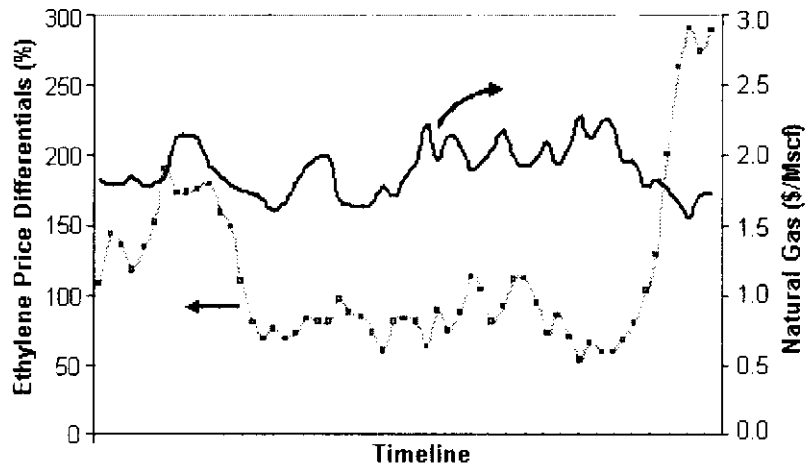
of Brent crude oil for a 60-month period between January 1990 and December 1994. Analysis of the price differentials reveals that, olefin and aromatic price differentials are always higher than the price differentials for gasoline. For example, the price differential for ethylene towards the end of the historical price trend is more than ten times higher than the price differential for gasoline. During these periods, producing ethylene is very profitable as compared to producing gasoline. Consequently, it can be expected that the demand for naphtha – a gasoline producing material - by liquid steam cracker plants would have also increased. The increase in demand is typically followed by an increase

in price. Figure 1.4 shows the changing price trend - which confirms the expectation - of naphtha price towards the end of the historical price trend. A similar price differential



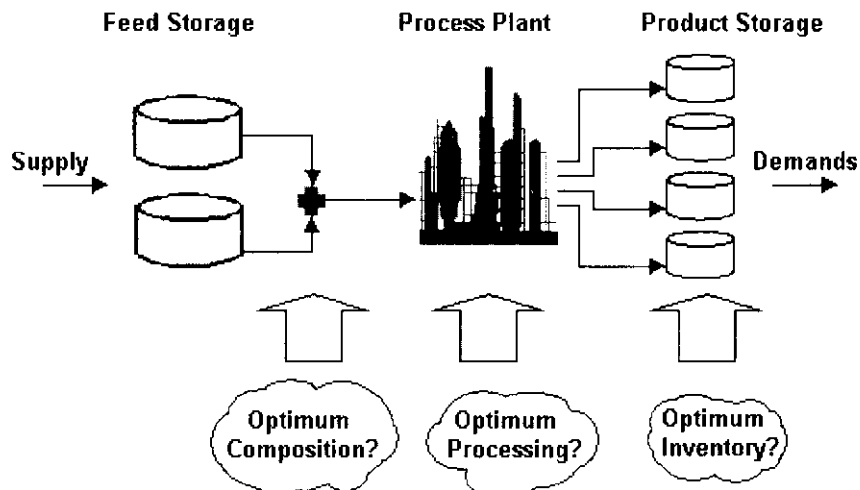
**Figure 1.4: A 60-month naphtha price trend**

analysis is performed for ethylene price differentials against the price of natural gas. The 60-month trend from January 1990 to December 1994 for the price differentials is shown in Figure 1.5. The price differentials for ethylene against the price of natural gas are also seen to increase towards the end of the trend period. Moreover, the trend for historical price of natural gas also shows a slower but increasing trend at the end of the 60-month period. During these periods, it is also expected that production of middle-distillates from natural gas would see a reduction in profit margins.



**Figure 1.5: Price differentials analysis against natural gas price**

To achieve the optimum operation at maximum profits, process plants must make the right decisions at various stages of production. As shown in Figure 1.6, decisions are made at different stages of the production process. Feeds purchased in the open market



**Figure 1.6: Decision Making in Production Planning Problem**

come with different qualities. The engineer must decide the optimum composition of feed mixture for the process plant. In addition, the process plant must also be operated at optimum conditions so as to maximise the profit while satisfying all product demands.

Products from the process plant are then stored in product storage tanks before delivery to the buyers. In oil refinery and petrochemical plants, customers' demands are typically focused to a small aggregate of products. It is possible that a considerable number of intermediate and low value products will be difficult to find sales. Unsold products generate inventory. Although some level of inventory for high saleable products is required as safety stock for future demand, other excess amount actually adds unnecessary cost to the production. Consequently, the engineer must also decide the optimum level of inventory.

All of these decisions are inter-related and complex. Moreover, these decisions contribute to the overall profitability for the process plant. For example, a change in feed composition will force a reactor unit to operate at different conditions resulting in different product distribution and different inventory profiles. It is therefore important to plan the productions efficiently by capturing the various synergies and trade-offs that exists at each decision stage.

The goal of production planning is to provide an efficient strategy to convert available plant resources into value added products. Production planning problem deals with operational decisions on what product to make, the quantity to make, the quality of the product, the selection of raw materials, and the parameters of process unit operations.

Planning decisions can be classified as strategic, operational, or tactical (Shobrys and White, 2000). The strategic planning is carried out over a long-term period of five years



or more. The aim is usually to identify the optimal timing, location and extent of investment required for process plant project. The operational planning is often short-term ranging from a period of few hours to a few weeks. The aim is to decide the optimal sequencing of a manufacturing task while accounting for the available resources and time constraints. The operational planning is also referred to as scheduling. The tactical planning addresses planning horizons of a few months to up to a few years. Tactical planning time periods are therefore set in between the time periods for the operational planning and the strategic planning. As a result, tactical planning usually incorporates some features from both the strategic and the operational planning. For example, the tactical planning accounts for carryover of inventory and various resource limitations at the beginning and the end of each production period much like scheduling decisions.

Production planning at the tactical level considers the processing units within its inside battery limit (ISBL) as well as the existence of various processing units that are located outside its battery limit (OSBL). The large scope also creates opportunity to integrate production with other plants, hence the main focus of this study.

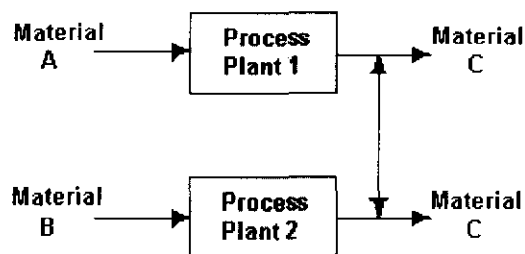
## ***1.2 Analysis and Optimisation of Integrated Production Planning***

The challenge in production planning is the uncertainty of what lies ahead in the future. Future prices, demands and performance of plants are unknown parameters. Nevertheless these parameters must be decided at the time of planning. What is decided now may

actually be different from what is several months later. As a result, production planning needs flexibility to adapt to changes in the future.

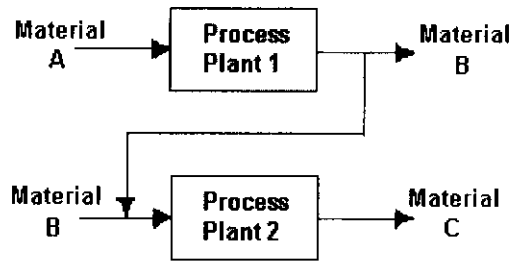
Among the three major attributes for any company to remain competitive are quality, cost, and time (Umble, et. al., 2003). In the case of oil and petrochemical industries, these plants are expected to produce higher quality product at the lowest cost and deliver to the customer in the shortest time. Technologies to address these issues have been developed. For example, process integration technology has been acknowledged to help lower the cost of production. Energy integration has been the key approach in process integration. In this work, the integration of materials will be analysed as another approach to reducing production cost. In addition, the flexibility of integrated production will also be addressed.

Integrated production can be classified according to the degree of interaction achieved. The lowest and simplest interaction involves only the exchange of final products. As shown in Figure 1.7, two plants that produce the same product can reduce their inventory cost by sending excess inventory of that product to the other plant. Product purity may be different. However, product purification, if needed, may be handled by the receiving



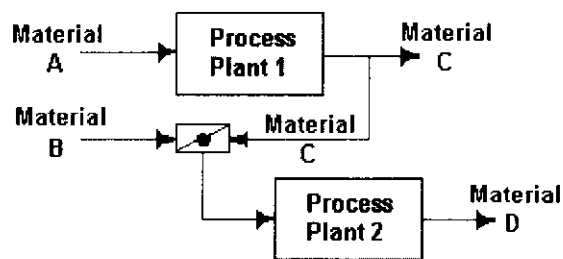
**Figure 1.7: Integration of final products**

plant using its existing product recovery section. At a higher degree, Figure 1.8 illustrates that a plant can also reduce excess inventory of intermediate products from another plant by using it as feed materials in its process unit. The quality of the material must be acceptable by the receiving plant and any upgrading, if required, must be carried out first.



**Figure 1.8: Integration of intermediate products**

The third degree of integration involves the sharing of a processing unit. Figure 1.9 shows that a plant can reduce its excess product inventory by sending its product to the other plant to be further processed into higher value products. Such an opportunity exists only when the processing unit is able to cope with different types of feed. Nevertheless, any upgrading of the materials should be carried out prior to feeding into the processing unit.



**Figure 1.9: Integration of processing unit**

### **1.3 Problem Statement, Aim and Objectives**

The oil refining and petrochemical industries are facing a challenging task to keep production cost competitively low on the back of globalisation and liberalisation of the commodity market where demand and prices are always uncertain. The extreme phenomena of globalisation is often associated with over production and dumping of products on one end to insufficient supply of raw materials and high feed price on the other end. This work proposes a solution to the problem through the strategy of integrated production. For complimentary plants like oil refineries and petrochemical plants, integrated production may provide the flexibility for sharing of resources and for co-production. Consequently, the strategy of integrated production may help to lower the impact caused by uncertainty in prices and demands. In addition, the potential cost savings can be realized through savings made on distribution costs. For integrated plants under the same financial management, savings on taxes is also possible.

The aim of this work is to explore issues of integrated production with respect to profitability, implementation and flexibility. Specifically, the following questions are raised:

- What is the impact of integrated production on an individual plant's profitability?
- When and how should the implementation of integrated production be carried out?
- Does integration increases plant's flexibility in the face of future uncertainty in demand and prices.

In achieving the aim, the objectives of this work are outlined as follows:

1. To develop models at process and site levels as well as an interaction model that represents an integrated oil refinery and petrochemical plant. These models further assist the evaluation of integrated production strategy for profit maximisation.
2. To develop procedures on how to systematically implement integrated production strategy. Issues with respect to computational difficulty and practicality will be addressed.
3. To develop a systematic method in assessing the impacts of price and demand uncertainty on costs and profits.

## ***1.4 Synopsis***

Chapter 2 presents the literature review of existing production planning methods. Limitations of such methods are addressed to indicate possible gap in knowledge.

Chapter 3 discusses model developments and problem formulations.

Chapter 4 discusses production planning models and the features of integrated production strategy. These features are highlighted through a case study example.

Chapter 5 discusses computational challenge to solving the NLP problem. Systematic approaches for efficient and practical solutions to integrated production problems are presented. A case study is presented to demonstrate application of the new approaches.

Chapter 6 discusses the uncertainty of prices and demand and its implication to production planning. It also highlights the flexible features of an integrated production strategy in minimising the impact of uncertainty. A case study is presented using the stochastic method to provide the scenario of integrated production under uncertainty.

Chapter 7 summarises and concludes the work. Plan for future work is also discussed.

## **1.5 References**

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## ***Chapter 2 Literature Review***

2.1 Review of Production Planning Problem.....	32
2.2 Flexibility of Production Planning.....	33
2.3 Integrated Production Planning.....	35
2.4 Gaps in Previous Works.....	37
2.5 References.....	38

## ***2.1 Review of Production Planning Problem***

The objective of production planning is to ensure that products are produced within the specified quantity and quality set by the company's management. The production must therefore operate in consistence with other performance measure as decided by the company. These measures include cost, profit, inventory level and process safety limit. A production plan states the quantity of each product to be produced period by period into the future defined as the planning horizon.

Crama et. al. (2001) provided a broad overview to production planning in process industries. The authors also found that mathematical programming provides a versatile tool to model and solve production planning problems. Ahmed and Sahinidis (2000) assessed the complexity of solving mathematical programming models for process planning with capacity expansions as the problem size increases. Production from a large number of different process plants have been typically described by linear models (Sahinidis et. al., 1989; Al-Sharrah, 2001; Al-Sharrah 2002). However, in their work, the authors did not address on the operational aspect of the process planning problem.

Timpe and Kallrath (2000) used mathematical programming to model and optimise the production planning of a chemical plant network. The production planning model features lot-sizing problems involving decisions on raw materials, production, inventories and demands. However, the use of linear models placed a realistic limitation on its application. Production planning of a refinery has been investigated by Moro et. al.



(1998) for the production of diesel. Non-linear models were used in searching for improvement in the single product and single period production campaign. A more complex refinery configuration has been studied by Pinto and Moro (2000) and Zhang (2000). The production planning optimisation problem is modelled and solved as an NLP problem for a range of products in a single period. Multi-product production planning greatly increases the number of decision variables in the optimisation problem. However, when only a single period is considered, the model suffers from a drawback of ignoring the elements of time and inventory. Both elements cannot be ignored because they add costs to the production. Neiro and Pinto (2004) expanded the scope of the planning model to cover the whole petroleum supply-chain. In this work, two time periods were considered. Multi-period and multi-product production planning was studied by Kiranoudis et. al. (1995) on a simple dehydration plant. Recently, Dave (2005) used a general decomposition strategy to solve the problem of optimising multi-period production planning for an overall refinery.

## ***2.2 Flexibility of Production Planning***

The future cannot be accurately predicted. At most, lessons learnt from the past would allow some forecast to be made. It is however not sufficient to eliminate uncertainty. As a result, a production planned for implementation at some point in the future is subjected to uncertainty. Uncertainty in production planning governs the price and availability of feed materials. It also affects the price and demand of products. For the production plan to be

successful, it must be flexible. Flexibility built into a production plan allows it to adapt to the changing future and continue to be feasible until the end of the planning horizon.

Grossmann and Sargent (1978) proposed a systematic approach to account for uncertainty in designing flexible processes. In their approach, a critical point within a range of uncertain design parameters such as pump efficiency and heat transfer coefficient is identified. It follows that if the design is found to be feasible over the critical point, then the design is flexible to operate feasibly within the entire region bounded by the uncertain parameters. Halemane and Grossmann (1983) later highlighted that there can be more than one critical point. Swaney and Grossmann (1985a, 1985b) further proposed the concept of flexibility index as a measure of the size of feasible region. These works however did not consider the effect of operational uncertainty such as variations in product demand and prices on the flexibility of the plant.

Pistikopoulos (1995) reviewed flexibility in both process design and process operations. Furthermore, the author proposed that uncertainty be treated as a component of flexibility. Sahinidis (2004) provided a comprehensive review of different methods of modelling and optimising production planning problems under uncertainty. The author showed that stochastic programming has been the most widely accepted and applied method. A variety of stochastic programming applications for production planning under uncertainty have been discussed by Ierapetritou et. al. (1996), Dantzig (1999), Hsieh and Chiang (2001), Gupta and Maranas (2003), Lababidi et. al. (2004), Li, W. et. al. (2004), and Li, P. et. al. (2004).

### ***2.3 Integrated Production Planning***

A refinery produces a number of streams for the production of fuel. Some of these streams can also be used directly as petrochemical feeds. The petrochemical plant can also return fuel byproducts to the refinery. Integrating refinery streams with petrochemical production benefits both plants by adding value and optimising their operations. Furthermore integrated production can also provide the means to buffer the plants against the uncertainty of future economic scenarios. As a result, the strategy of integrated production increases the flexibility for the production planning to respond and adapt into a new point of operations.

Bhatnagar et. al. (1993) discussed issues in the implementation of integrated production between different plants in a vertically positioned manufacturing industry. For the process industry, the earliest discussion found for integrated production between an oil refinery plants and a petrochemical plant was given by Sloley (1994). The author proposed for sharing of propylene products between the refinery's fluid catalytic cracker unit and the steam cracker unit in a petrochemical plant. Propylene is a major byproduct of the two process units. Sadhukan (2001) performed value analysis for a proposed process network involving the integration of refinery with petrochemical productions. The author performed systematic selection of best processes for integration. Swaty (2002) explored the opportunities for substantial economic benefits through the integration between a refinery's hydrocracker and proximate petrochemical steam cracker plant. Furthermore, the integration is modelled as an LP problem. Ota. et. al. (2002) discussed

the integration of aromatic rich pygas between steam crackers in a petrochemical plant and benzene production units in an aromatic plant. The problem was solved for an optimum blending of naphtha feed into the steam cracker.

Many large oil and chemical companies are currently putting the idea of integrated production into practice. Potential substantial economic returns are possible for refineries and proximate ethylene plants that can actively interchange intermediate streams. For this reason, French-based TotalFinaElf and German's BASF have constructed an integrated oil refinery and petrochemical plant on adjacent site in Port Arthur, Texas, USA (Antosh, 2001). These companies foresee integration of various productions as a key strategy in cutting operations cost and improving plant efficiency (Hairston, 2001). Mitsubishi Chemical Company has commissioned Optience Corporation to study optimum management of enterprise-wide planning in the petrochemical industry. The company emphasised the need to have a single higher level system that would be able to make decisions for an integrated production planning (Tjoa et. al., 2004). Shell International Chemicals and its subsidiary Shell Global Solutions have also developed a management approach to screen for integrated production opportunities between the company's oil and petrochemical plants (Moorthamer, et. al., 2004).

## ***2.4 Gaps in Previous Works***

The interest in developing integrated production has grown since the turn of the new millennium. This is probably due to companies realising the increasing threat of competing in a globalised economy and the need to sustain their businesses. Despite the development, there are still numerous gaps in the research on integrated production for oil refineries and petrochemical plants.

Firstly, due to the size of the problem, many integrated production models are built using linear formulation. Linear models suffer from lack of accuracy in representing non-linear processes such as the fluid catalytic cracker, the catalytic reformer and the steam cracker. In this work, the non-linearity of the process will be preserved and solution strategies will be developed to handle the complexity of non-linear programming.

Secondly, some studies focused only on single product integration between two processing units in the integrated plants. In this work, the proposed integrated production strategy will attempt to explore several options for network integration.

Finally, majority of the study on integrated productions are carried out by the industries themselves. On one hand, this phenomenon is probably due to the size and complexity of the problem that is just too large for academic research. On the other hand, the industry practitioners are probably secretive to talk about their production strategies openly with

the academia. This work will attempt to explore issues related to the integrated production using as much available resources as there is in open literatures.

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## **Chapter 3 Modelling Strategy**

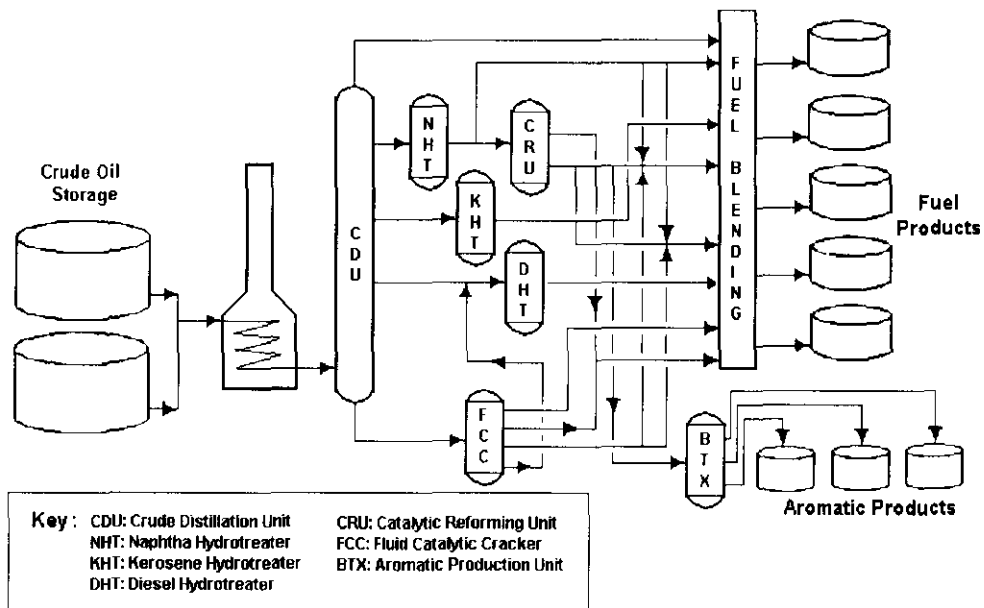
3.1 Introduction.....	43
3.2 Site Level Modelling.....	46
3.2.1 Mixer Model.....	49
3.2.2 Splitter Model.....	50
3.3 Process Level Modelling.....	50
3.3.1 Crude Distillation Model.....	51
3.3.2 Hydrotreaters Model.....	52
3.3.3 Catalytic Reformer Model.....	53
3.3.4 Fluid Catalytic Cracker Model.....	55
3.3.5 Aromatic Production Model.....	57
3.3.6 Steam Cracker Model.....	59
3.3.6.1 Development of Steam Cracker Model.....	59
3.4 Overall Formulation.....	65
3.5 Summary.....	67
3.6 References.....	68

### **3.1 Introduction**

The aim of production planning process is to make operational decisions on the allocation of raw materials to the processing units, the operating conditions of each processing unit, and the distribution of products. The challenge is how to make these decisions in the most cost effective way under the constraints of demands and process limitations. It is even more challenging when demand and prices are not always certain. Production plan therefore needs the flexibility to adapt to changing scenarios in the future.

This work presents a method of creating flexibility in production planning process by integrating production plans between two complementary plants. Complementary plants refer to plants that share similar materials in their feed, intermediate or final products. Two examples are an oil refinery and a petrochemical plant.

The oil refinery and the petrochemical plant modelled in this work are assumed to be sited adjacent to one another. Figure 3.1 shows a typical oil refinery flowsheet. It consists of various processing units to fractionate the crude and to hydrotreat, reform and crack the crude oil components into various products. There is also a small aromatic production facility situated within the battery limit of the oil refinery. The refinery receives two types of crude and produces a set of 11 products that can be classified as fuel, intermediate, olefin, and aromatic.

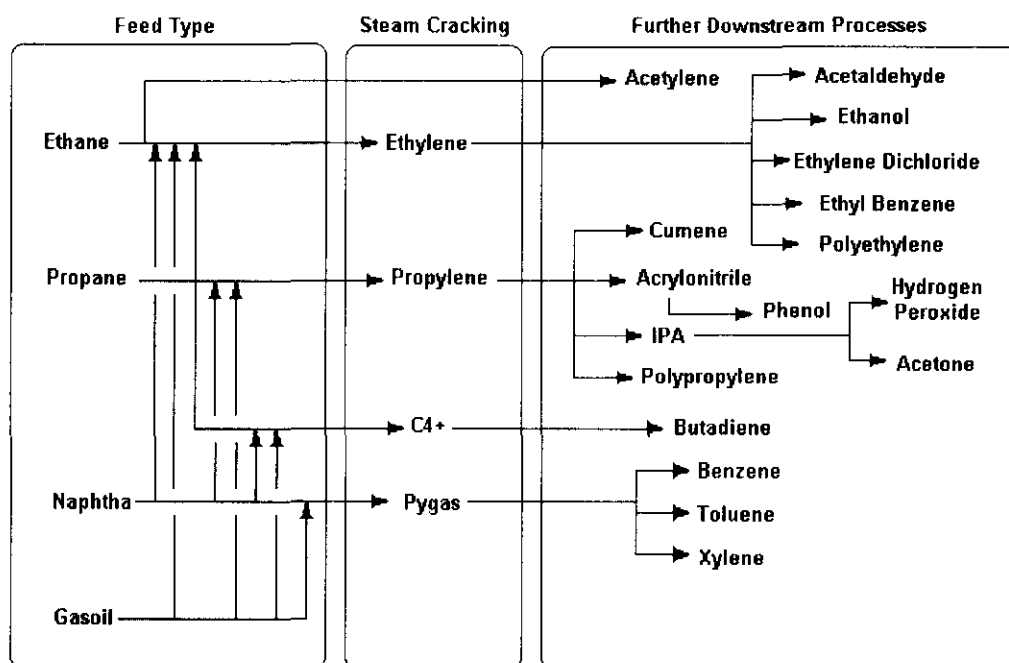


**Figure 3.1: An oil refinery flowsheet incorporating an aromatic production unit**

Other than an oil refinery, a petrochemical plant is also modelled. A petrochemical plant complex can generally be divided into upstream and downstream processes. Upstream petrochemical processes manufacture basic chemicals such as C2 and C3 olefins and other less valuable byproducts such as pygas and fuel oil. The downstream processes further use the basic chemicals to manufacture a multitude of petrochemical products ranging from intermediate chemicals to plastics.

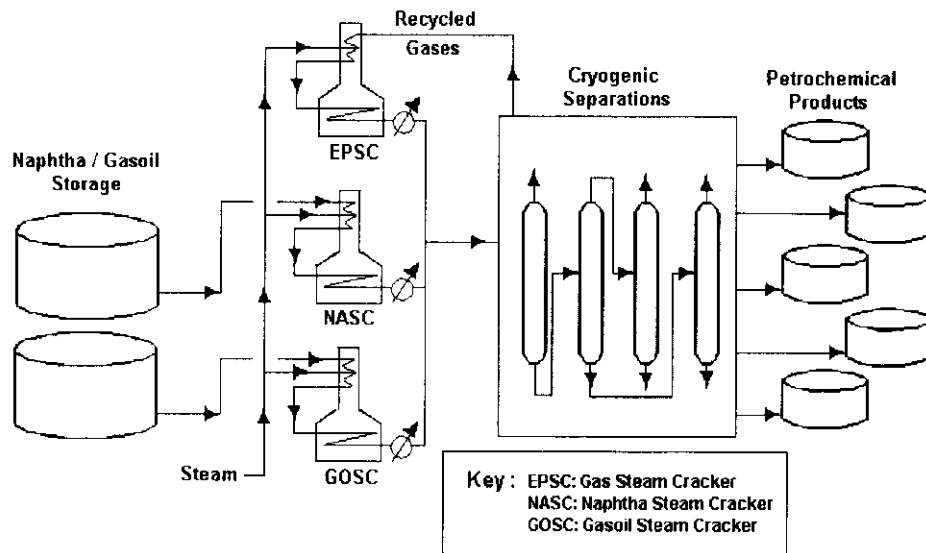
The range of processes that exist under a petrochemical plant complex is illustrated in Figure 3.2. To model the whole range of a petrochemical plant complex is indeed a huge task. Since complete coverage of the whole petrochemical complex may be impractical, this work proposes that some limitation of scope is required. The size of the petrochemical plant model can be greatly reduced by recognising that only the steam

cracking process carries significant potential for materials integration between an oil refinery and a petrochemical plant. Consequently, only upstream steam cracking processes are modelled. All further downstream derivative petrochemical processes are neglected in this work.



**Figure 3.2: General outline of a petrochemical plant complex**

The petrochemical plant flowsheet used in this work is shown in Figure 3.3. The steam cracker model comprises two liquid crackers and one gas cracker. The liquid crackers run on naphtha and gasoil feeds. The gas cracker is a small unit that takes in recycled ethane and propane from the cryogenic separation unit. Within the cryogenic separation unit are various sub-ambient distillation processes that separate fractions of C1 and lighter, C2 paraffin and olefin, C3 paraffin and olefin, C4, and C5 along with components heavier than C5. The petrochemical receives naphtha and gasoil from tank farms and produces a set of six products that can be classified as olefins, intermediate/fuel and fuel.

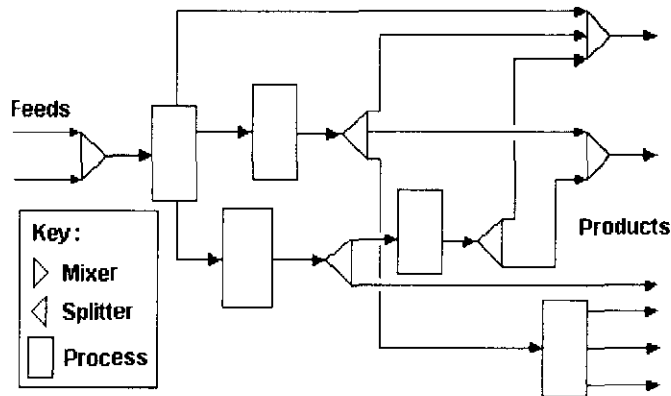


**Figure 3.3: A petrochemical plant flowsheet for the production of basic chemicals**

The two flowsheets illustrated in Figure 3.1 and Figure 3.3 are modelled to provide the basis for integrated production planning strategy. Each flowsheet is modelled in two aspects. First, the site level model which describes the overall materials flow into and out of the plant. The second aspect of the model mimics the individual process unit which converts feed at a given quality into products at some operating conditions.

### **3.2 Site Level Modelling**

A plant configuration can be generally described as a number of process units linked by splitters and mixers. Each process unit contains several unit operations such as reactors, separators and heat exchangers. Figure 3.4 shows an example of a generalized plant configuration.



**Figure 3.4: A generalized plant configuration**

Revenue can be calculated from revenue generated streams (i.e. streams carrying materials that are saleable)  $F_j$  for any period  $t$  as follows:

$$R_t = \sum_j c_j F_{j,t} \quad (3.1)$$

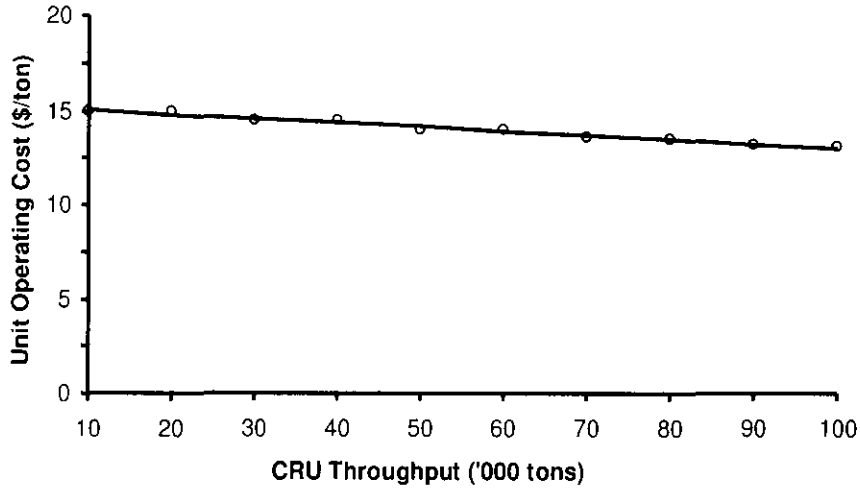
The term  $c_j$  refers to unit price of any output material  $j$ .

Production costs are also incurred from the plant. These costs comprise the cost from cost incurred streams, the cost of process unit operations and the cost of product inventories. Firstly, the cost from cost incurred streams  $F_i$  for any period  $t$  is written as:

$$CM_t = \sum_i c_i F_{i,t} \quad (3.2)$$

The term  $c_i$  refers to unit price of any input material  $i$ . Secondly, the cost of process unit operations is typically made up of utilities, labours and miscellaneous overhead costs. Moreover, these costs are significantly affected by variations in process unit throughputs. Estimates for these costs on many process units are readily available in the

literatures. Figure 3.5 shows an example of the correlation between the unit operating cost and the throughput of a catalytic reforming unit (UOP, 2003). Cost data for process unit operations is shown in **Appendix A**.



**Figure 3.5: Unit operating cost as a function of process unit throughput**

It follows that for any process unit  $n$  operating at throughput  $Q_n$ , the cost incurred from process operations is:

$$CP_t = \sum_n c_{OP,n} Q_{n,t} \quad (3.3)$$

Finally, product inventory generates cost when the quantity of any product  $i$  surpasses its' demand. Until the next demand appears, the current product has to be stored. The quantity of inventory,  $QI_i$ , at any time  $t$  is therefore defined as the difference between the quantity produced,  $F_j$ , and its demand,  $D_j$ , add any amount of product already in inventory from the last period of production  $t-1$ . This is mathematically shown in Equation (3.4) below:

$$QI_{j,t} = QI_{j,t-1} + F_{j,t} - D_{j,t} \quad (3.4)$$



Determining the cost of product inventory is difficult. The cost of inventory is typically made up of the capital and operating cost for the storage facility as well as administrative cost, cost of insurance and taxes. Many industries use a rule of thumb that varies between 20% and 29% of the product value (Schreibfeder, 2003; Timme and Williams-Timme, 2003; Martin, 2004). In this study, we consider the cost of holding product inventory at 25% of its value. Hence for any product  $j$  in inventory, the cost of inventory is written as:

$$CI_t = \sum_j c_{ij} QI_{j,t} \quad (3.5)$$

where  $c_{ij}$  is the unit cost of inventory for product  $j$ .

The total cost of production is a summation of Equations (3.2), (3.3) and (3.5). Moreover, the difference between Equation (3.1) and the total cost of production gives the profit generated from plant production.

### **3.2.1 Mixer model**

A mixer sums all inlet streams as a single output stream. The flow of the output stream at any time  $t$  is given by the mass balance equation as follows:

$$F_{j,t} = \sum_i F_{i,t} \quad (3.6)$$

In addition, the physical properties,  $\gamma$ , and chemical compositions,  $\zeta$ , of the output stream can be found by weighting the average physical property and chemical

composition of each inlet stream. These are described mathematically in Equation 3.7 and Equation 3.8.

$$\gamma_{j,t} = \sum_i \gamma_i F_{i,t} \quad (3.7)$$

$$\zeta_{j,t} = \sum_i \zeta_i F_{i,t} \quad (3.8)$$

### **3.2.2 Splitter model**

A splitter is modelled with one inlet flow and a number of outlet flows. The total mass balance around a splitter at any time  $t$  is given by

$$\sum_j F_{j,t} = F_{i,t} \quad (3.9)$$

Unlike a mixer, the flow through a splitter encounters no physical or chemical change.

## **3.3 Process Level Modelling**

Within each process unit that makes up a plant configuration, there are a number of specific unit operations  $n$ . Process level modelling is required to describe process performance (e.g. yields, operating costs) related to the operating conditions (e.g. temperatures, pressures, conversions) in specific unit operations as the operating conditions change. By combining process models into site models, an overall economics decision of the plant production can be made.

A unit operation  $n$  consists of a set of inlet flow  $i \in F_{i,n,t}$ . These flows have a set of physical properties  $\gamma_{i,n,t}$ . Similarly there are also a set of outlet flows  $j \in F_{j,n,t}$  with corresponding physical properties  $\gamma_{j,n,t}$ . The mass balance for each product flow  $j$  and its physical properties at any operating conditions  $\phi_{n,t}$  and time  $t$  are given by

$$(F_{j,n,t}, \gamma_{j,n,t}) = f(F_{i,n,t}, \gamma_{i,n,t}, \phi_{n,t}) \quad (3.10)$$

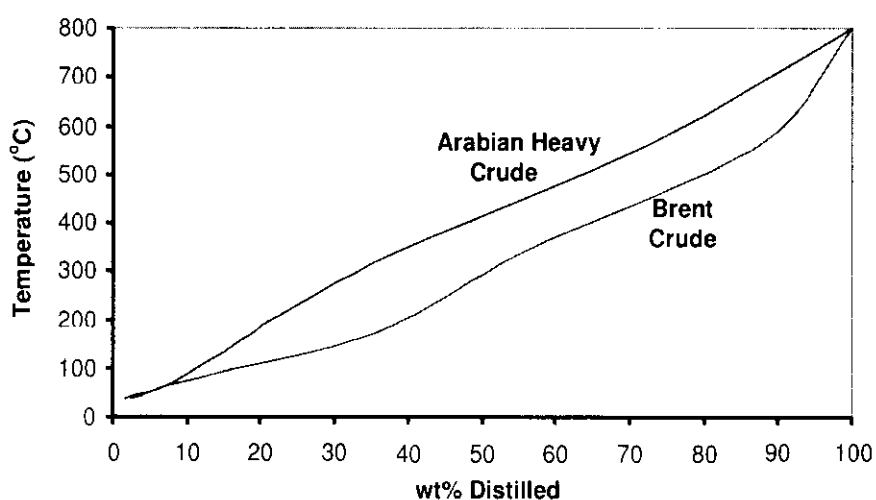
The formulation of  $f(F_{i,n,t}, \gamma_{i,n,t}, \phi_{n,t})$  depends on the mechanics behind individual processes. This formulation is usually represented by a set of equations describing the kinetics, thermodynamics, and/or hydrodynamics of the unit operations. Moreover, these equations are typically non-linear.

The following sections discuss major process models in an oil refinery and a petrochemical plant used in this work.

### **3.3.1 Crude Distillation Model**

The crude distillation model is presented by a series of yield structure for each crude type. Each crude type has unique cut points. These cut points follow a general crude assay system with yields and properties generated from laboratory true boiling point or TBP distillation. TBP distillation separates the crude oil at atmospheric and also in vacuum pressure into a range of product yields in accordance with the ASTM standards. Crude assay systems are periodically published by oil companies in the companies' publications or in professional oil and gas journals.

TBP distillation curves for two types of crude are illustrated in Figure 3.6. Arabian Heavy crude is heavier than Brent crude. This explains why Arabian Heavy crude produces more than 20% higher kerosene and heavier fractions (cut point higher than 220°C) than the Brent crude. The crude distillation model used in this work is shown **Appendix B1**.



**Figure 3.6: TBP Curves for Heavy (Arabian Heavy) and Light (Brent) Crudes**

### ***3.3.2 Hydrotreaters Model***

Hydrotreaters are used to remove sulfur and nitrogen compounds under mild operating conditions. The maximum operating temperature and pressure of a hydrotreater are typically below 400°C and 50 bar, respectively. Consequently, the operation of a hydrotreater hardly affects the boiling range of its feed. Hydrotreaters are used to treat naphtha, kerosene, diesel and gasoil. These products require the content of sulfur and

nitrogen compound to be below a maximum limit. For example, the limit of sulfur in diesel set by the European Union is currently 500 ppm.

Models to predict yields from hydrotreaters are adopted from HPI correlations (Baird, 1987). Key correlation parameters are sulfur and nitrogen contents in feed as well as the specific gravity of feed ( $SG_f$ ). The correlation is also non-linear with respect to  $SG_f$ .

### **3.3.3 Catalytic Reformer Model**

Catalytic reformer converts low-octane naphtha range feed into high-octane reformate. Reformate is used as blend stocks to increase the quality of gasoline products. This work uses HPI correlations (Baird, 1987) to model the catalytic reformer. Two important parameters that affect the yield are the quality of feed and the operating conditions of the catalytic reformer. The quality of feed is expressed in terms of the specific gravity of feed ( $SG_f$ ) and the amount of naphthene plus two times the amount of aromatic in feed ( $N2A$ ). Furthermore, the operating condition is expressed in terms of the operating pressure ( $P$ ) and the severity of the catalytic reformer operations. Severity is characterised by the research octane number ( $RON$ ) of the resulting reformate product.

The catalytic reformer model is nonlinear with respect to  $N2A$  and  $RON$ .  $N2A$  affects the amount of aromatics produced through dehydrogenation of naphthenes to aromatics and the dealkylation of higher aromatics. Figure 3.7 shows that, for a fixed

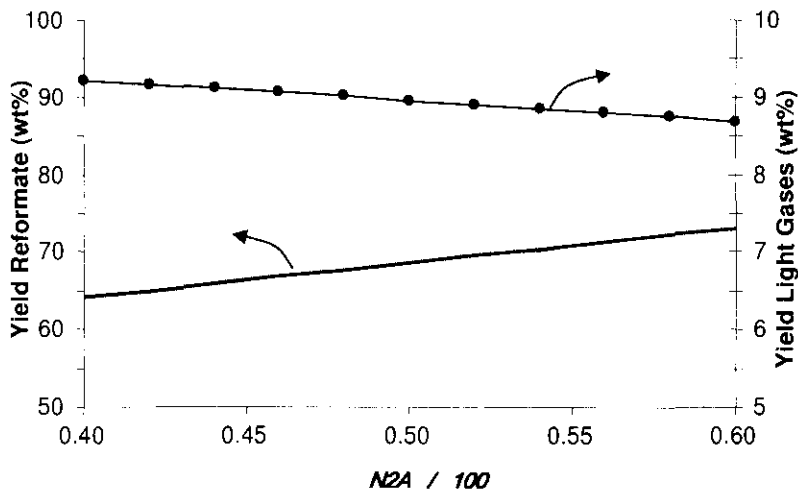


Figure 3.7: Reformate yield as a function of *N2A*

pressure and severity, greater reformate and lesser light gases will be produced as the amount of naphthene and aromatic increases in feed. However, unlike *N2A*, higher *RON* increases the quality of reformate at the expense of quantity. As shown in Figure 3.8, for fixed reformer pressure and feed quality, higher *RON* produces less reformate

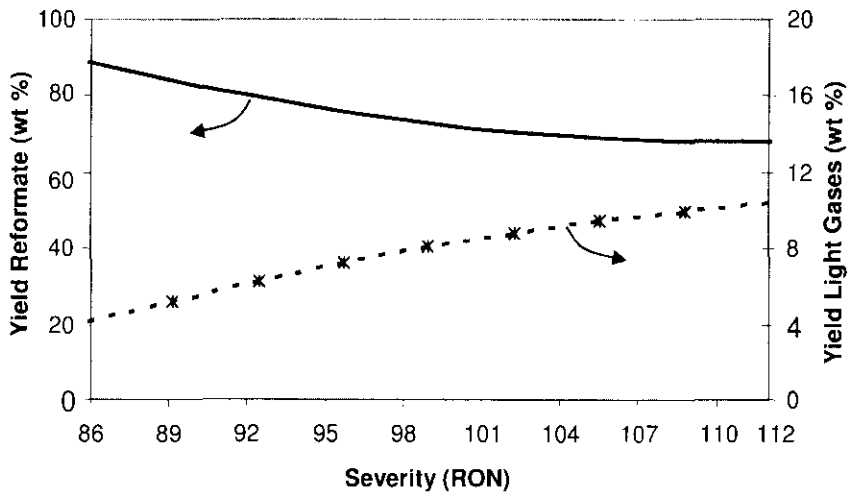


Figure 3.8: Reformate yield as a function of *RON*

and generates more light gases. In this work, the trade-off between quality and quantity of reformate is treated as an optimisation problem.

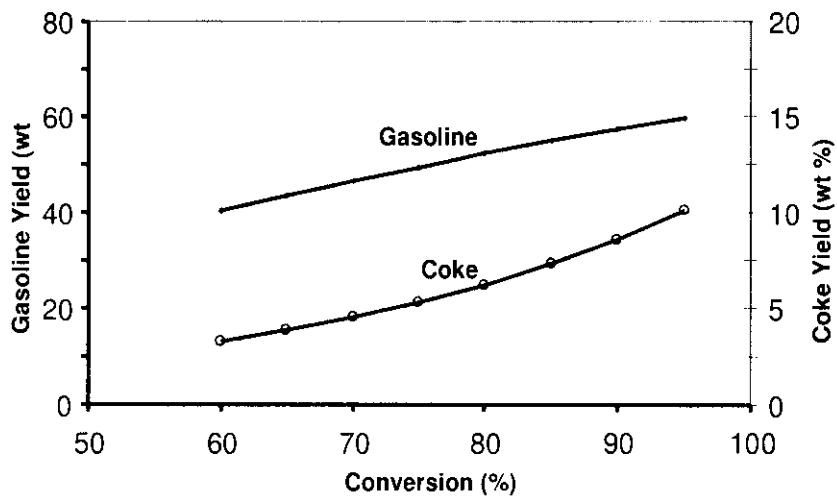
### 3.3.4 Fluid Catalytic Cracker Model

Fluid catalytic cracker (FCC) plays an important role in enhancing the economics of an oil refinery. FCC upgrades low-value heavy oils input into high value gasoline range output. In this work, the model for FCC unit is adopted from HPI correlations (Baird, 1987).

The yield from FCC is correlated to two key variables. The first variable is the level of FCC conversion. The second variable is the feed quality parameter or **FQP**. **FQP** is a variable used to describe the quality of the feed into FCC. It is calculated as follows:

$$FQP = f(SG_f, VABP_f, S_f, AP_f) \quad (3.11)$$

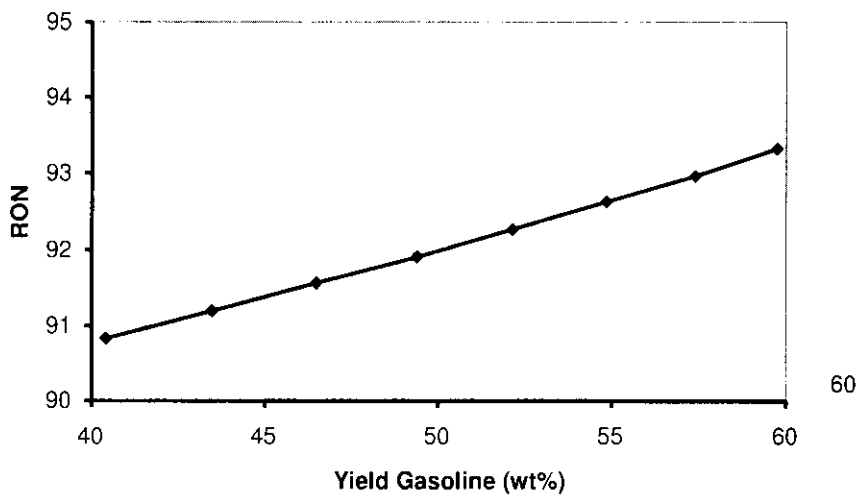
In Equation 3.11, the parameter **SG<sub>f</sub>** refers to the specific gravity of the feed, **VABP<sub>f</sub>**, the volumetric average boiling point of feed, **S<sub>f</sub>**, the amount of sulfur in feed, and **AP<sub>f</sub>**, the feed aniline point temperature. Aniline point is correlated to the amount and type of aromatic hydrocarbons in the feed. A low **AP<sub>f</sub>** value is indicative of high aromatics, while a high **AP<sub>f</sub>** value is indicative of low aromatics content in feed.



**Figure 3.9: Effect of FCC conversion on gasoline and coke yields.**

The FCC model is non-linear with respect to conversion and *FQP*. Figure 3.9 shows the effect of reactor conversion on the yield of gasoline and the formation of coke.

Furthermore, as shown in Figure 3.10, high gasoline yield is also associated with



**Figure 3.10: Gasoline RON as a function of yield.**

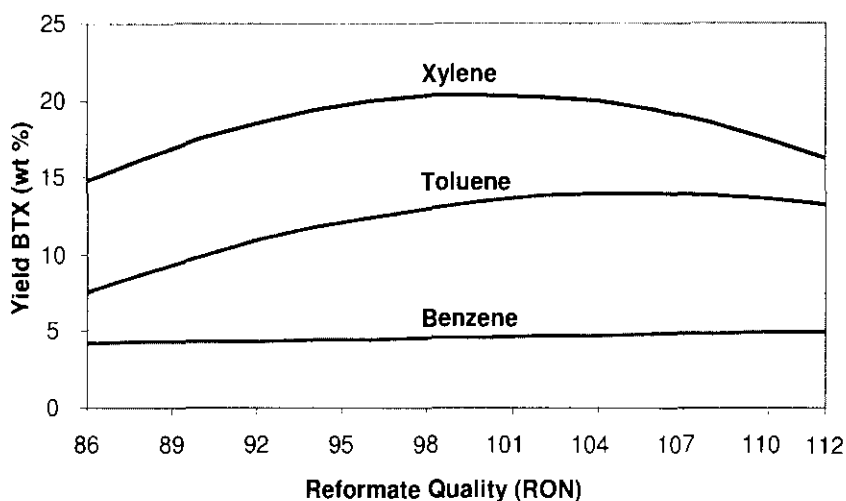


increases in the gasoline octane number. While high conversion is beneficial because both the yield and the quality of gasoline increases, it is however unfavourable to operate at a very high conversion level due to the exponential increase in coking. Typical upper coking level is about 8 wt% corresponding to around 90% FCC conversion.

### **3.3.5 Aromatic Production Model**

Aromatic production is a major process unit for the manufacture of benzene, toluene and xylene (BTX). BTX are basic aromatic building blocks for the manufacture of styrene, caprolactam and terephthalic acids.

BTX are obtained through extraction from aromatic rich feedstock. Reformate from catalytic reformer provides a major aromatic feedstock from oil refinery. Peng (1999) developed a molecular model of catalytic reforming unit that was able to describe the molecular distributions of the reformate product. In this work, the molecular model by Peng (1999) was used to correlate the yield of BTX to two key variables used in HPI correlations (Baird, 1987) for catalytic reforming unit. The key variables are ***N2A*** and ***RON***. ***N2A*** refers to the quality of feed into the catalytic reforming unit while ***RON*** refers to the quality of the reformate product. Figure 3.11 illustrates the nonlinear effect of ***RON*** on the contents of BTX in the reformate.

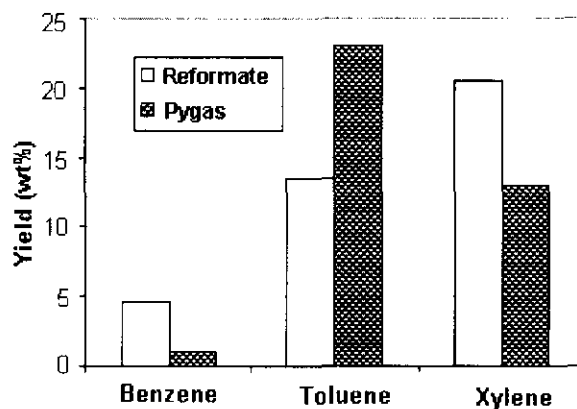


**Figure 3.11: Effect of reformate quality on BTX yield**

Higher **RON** is associated with lower yields of xylene and toluene. This is explained by the higher severity of reformer operations which causes dealkylation of high molecular weight aromatics.

Another source of aromatic feedstock is available from pygas. Pygas is a byproduct of steam cracking for the production of olefins in the petrochemical plants. However, the aromatic quality in pygas is lower than that in reformate. Pygas normally requires olefins saturations and desulphurisation before it is sent for aromatic extractions. In this study, BTX yield from pygas is modelled linearly. Figure 3.12 illustrates a typical comparison of BTX yields extracted from reformate (**RON** = 100, **N2A** = 50) and pygas feedstocks. In this example, the reformate feedstock shows a distinctively higher benzene and xylene yields while the pygas feedstock shows higher toluene yield.

The aromatic production model used in this work is shown **Appendix B2**.



**Figure 3.12: Comparison of BTX yields from reformat and pygas**

### **3.3.6 Steam Cracker Model**

The steam cracker is the primary process unit for the production of petrochemicals such as ethylene and propylene. These products form the basic olefinic building blocks for many other downstream petrochemical and polymer products. Much of the reported work in building steam cracker models uses either molecular or mechanistic approaches (Sundaram and Froment, 1977a,b; Kumar and Kunzru, 1985; Dente et. al., 1979 ). While these models are highly accurate, they are unfortunately too computationally demanding to be easily incorporated into the overall formulation for the production planning optimisation problem. Hence, this work proposes a simple correlation approach to model the yield of a steam cracker.

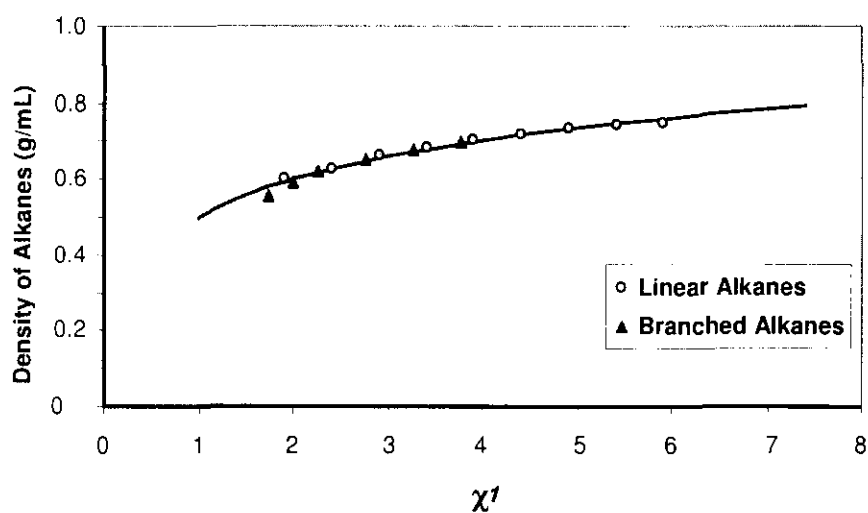
#### **3.3.6.1 Development of Steam Cracker Model**

The distribution of steam cracker products has been observed to vary with the type of feedstock and the operating conditions of the steam cracker unit (United Nations, 1971).

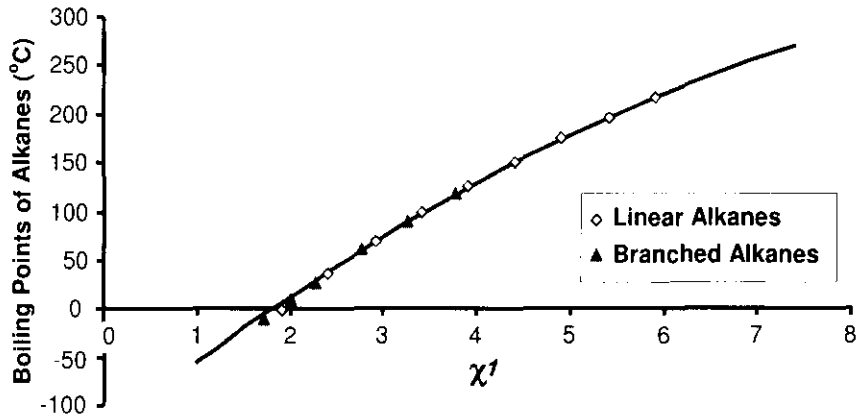
The quality of the feedstock is a characteristic of its molecular composition. Randić (1975) proposed a technique to quantify the relations between the structure of a molecule and its property by accounting for the degree of branching in the molecule. This relation is called Randić index ( $\chi^1$ ) and it is expressed mathematically as,

$$\chi^1 = \sum_{(i,j) \in E} \frac{1}{\sqrt{V_i V_j}} \quad (3.12)$$

The index is calculated by accounting the number of consecutive edges  $E$  in a given molecule. These edges form the paths between any two adjacent vertices  $V_i$  and  $V_j$ . As shown in Figures 3.13 and 3.14,  $\chi^1$  shows excellent correlation to the density and



**Figure 3.13: Correlations between density of alkanes and  $\chi^1$**



**Figure 3.14: Correlations between boiling points of alkanes and  $\chi^1$**

boiling point of linear and branched alkanes. Consequently, it is possible to predict the properties of hydrocarbons if the molecular composition of those hydrocarbons is known.

For complex hydrocarbon feedstocks comprising paraffins, olefins, naphthenes, and aromatics (PONA), a molecular index,  $I_M$ , is proposed.  $I_M$  is defined as the sum of the weighted average of pure component's  $\chi^1$  as follows:

$$I_M = \sum_i x_i \chi_i^1 \quad (3.13)$$

In Equation 3.13 above,  $x_i$  represents the fraction of component  $i$  in the mixture. The molecular index method is also very convenient to characterise the quality of a given feeds assay as described by a Molecular Type Homologous Series (MTHS) matrix (Peng, 1999).

Another important parameter affecting the yield distribution of steam cracker is the cracking severity. Cracking severity varies with the coil temperature, the residence time

and the partial pressure of hydrocarbon in the reactor. Zdonik et. al. (1968) proposed kinetic severity factor (KSF) which is determined from the rate of decomposition of n-pentane against the residence time. Later, Shu and Ross (1982) proposed cracking severity index (CSI) which is determined from the yield of C3 and lighter gases. Mallinson et. al. (1992) noted that pressure effect on rate of reactions is only significant either at very low or very high pressure. In this work, the operating pressure is assumed to be slightly above atmospheric. Hence pressure effect is neglected.

In this work, severity index,  $I_S$ , is proposed.  $I_S$  is defined as the rate at which a given hydrocarbon feedstock decomposes as it travels along the space-time of the cracking coil.

$$I_S = \kappa\theta \quad (3.14)$$

In Equation 3.14,  $\kappa$  is Arrhenius rate constant for the hydrocarbon feeds in  $s^{-1}$  and  $\theta$  is the residence time in s. Pre-exponential factor and activation energy for the steam cracking of gaseous and liquid hydrocarbons are available from the literature (Sundaram and Froment, 1977a,b; Kumar and Kunzru, 1985).

Both the molecular index and the severity index form the key variables in the steam cracker model developed in this work. The proposed model is regressed against industrial and experimental data for ethane/propane (Ross and Shu, 1977) and naphtha steam cracking (Goossens et. al., 1978). The coil outlet temperature for these operations varies from 780 to 860°C. Furthermore, the residence time ranges between 0.3 and 1.4 s. Figures 3.15 and 3.16 show the parity plot between the predicted and observed yields of

ethane-propane and naphtha steam cracking. The correlation coefficients for the plots are 97.1% and 93.2% respectively.

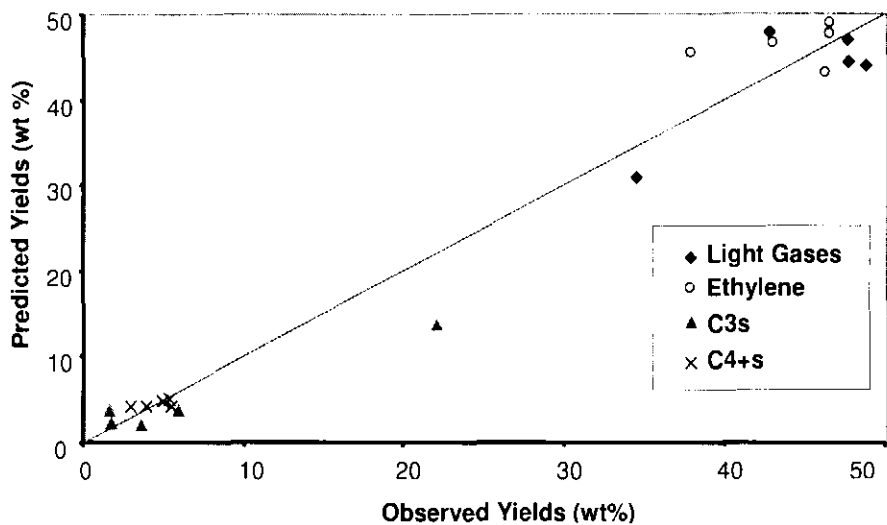


Figure 3.15: Parity plot for Ethane-Propane Correlation Model

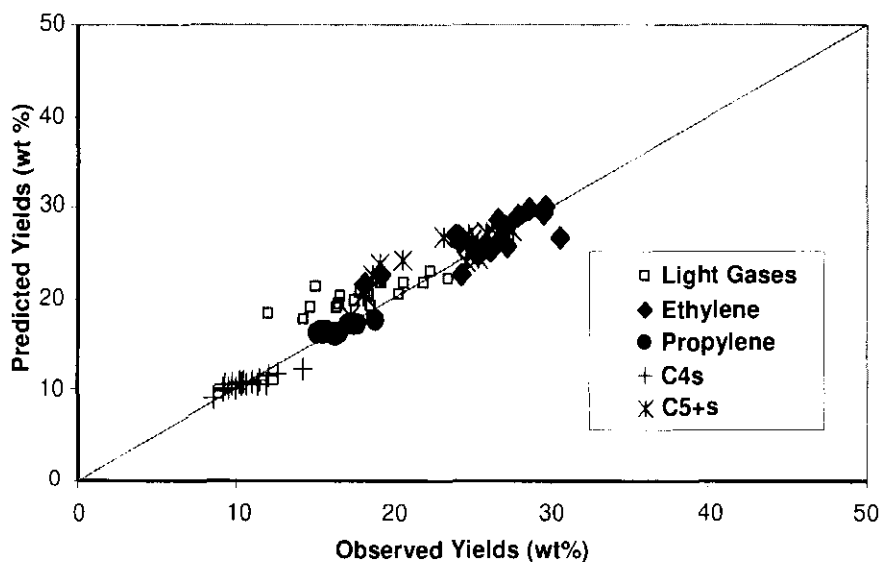
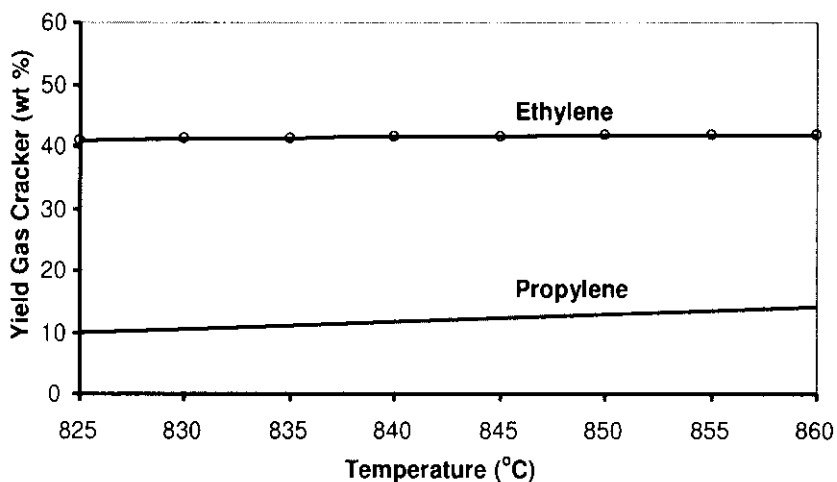
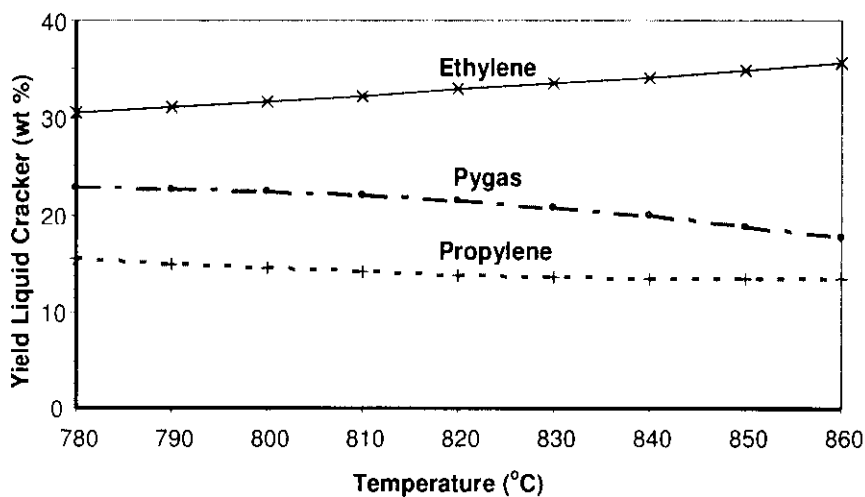


Figure 3.16: Parity plot for Naphtha Correlation Model

The steam cracker model developed in this work is able to describe the pattern of production from both gaseous and liquid steam cracker with reasonable accuracy. Their simplicity results in less computational effort than that required by either the molecular or the mechanistic models. Figures 3.17 and 3.18 show the yield patterns of some major



**Figure 3.17: Model prediction for the steam-cracking of 80/20 ethane-propane feed at varying temperature and fixed residence time of 0.35 s.**



**Figure 3.18: Model prediction for the steam-cracking of heavy naphtha feed at varying temperature and residence time of 0.35 s.**



products from the gaseous and liquid steam crackers. In both cases, residence time was fixed at 0.35 s. The predicted yields of ethylene, propylene and light gases in Figure 3.17 are within the range reported by Ross and Shu (1977). The predicted yields for liquid steam cracker products are somewhat low but are still within the range reported by Goossens et. al. (1978).

Correlations for steam craker productions are shown in **Appendix B3**.

### 3.4 Overall Formulation

Given a multi-product process plant, the cost of producing any product is made up of the cost of feed materials and the production cost involved in operating the process units that convert feed into products. It is also expected that some products will be overproduced. Keeping unsold product in inventory is an added cost to the production. As a result, the total cost, **CT**, is a combination of three components shown mathematically below,

$$CT = \sum_t (CM_t + CP_t + CI_t) = \sum_j \sum_t c_j F_{j,t} + \sum_n \sum_t c_n Q_{n,t} + \sum_j \sum_t c_{ij} QI_{j,t} \quad (3.15)$$

In equation 3.15, the terms **CM**, **CP**, and **CI** refer to, respectively, the cost of raw materials, the production cost, and the cost of product inventory as per equations (3.2), (3.3) and (3.5). Furthermore, the profit generated is estimated from the following equation,

$$Profit = RT - CT = \sum_j \sum_t c_j F_{j,t} - \sum_j \sum_t c_j F_{j,t} - \sum_n \sum_t c_n Q_{n,t} - \sum_j \sum_t c_{ij} QI_{j,t} \quad (3.16)$$

There are two major constraints to the problem above. The first major constraint is dictated by the demand. In this work, the demand is a hard constraint as no back-order is allowed. This means that all demand of product  $i$  during period  $t$  must be met before the end of that period. This is ensured by setting the inventory constraints to be non-negative as follows:

$$QI_{i,t-1} + F_{i,t} - D_{i,t} \geq 0 \quad (3.17)$$

Equation (3.17) can also be adjusted to account for materials flow between two or more plants during period of integrated production.

The second major constraint arises from the yield relations between feeds and products. These relations are process specific. They typically correlate to different feeds and different process operating conditions. Process operating conditions introduce nonlinearity through the expressions of feed conversion or reaction severity. Thus the overall problem is modelled as an NLP.

Other constraints for the problem above include physical bounds, product specifications and the nonnegative constraints on yields and materials flow. Thus the following equations are used.

Physical bound of process unit  $n$ ,

$$Q_n^L \leq \sum_i F_{i,t} \leq Q_n^U \quad (3.18)$$

Minimum quality specification for product  $j$ ,

$$\gamma_{j,t} \geq \gamma_j^L \quad (3.19)$$

Non-negative constraints for product  $j$ ,

$$F_{j,t} \geq 0 \quad (3.20)$$

### **3.5 Summary**

In this chapter, a general modelling strategy for overall production planning optimisation is developed. The model consists of an overall planning at the site level and individual yield correlations at the process level. Yield correlation models are simple yet sufficiently accurate to predict the production profiles of both oil refinery and petrochemical plant processes. An advantage of this modelling strategy is that plant economics at the site level can be calculated and improved through repeated access of the yield correlation model at the process level. Another advantage is that generation of materials flow between plants for integrated production at the site level can be carried out by judicious selection of material flows from available units at the process level. Hence, the formulation of complex production planning problem in this work is simplified without losing the details of characteristics of production but the proposed model is effective to solve using reasonable computing resource.

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## **Chapter 4 Planning for Integrated Production of Oil Refinery and Petrochemical Plant**

4.1 Introduction.....	71
4.2 Hierarchy of Production Planning Process.....	71
4.3 Production Planning Models.....	73
4.4 Features of Integrated Production Planning.....	77
4.4.1 Modelling Integrated Production.....	79
4.5 Case Study: Integrated oil refinery and petrochemical production for profit maximisation.....	81
4.6 Summary.....	90
4.7 References.....	91

## ***4.1 Introduction***

Production planning involves the decision making at various stages of production. One objective of a production planning process is to increase the profit margin of the plant. In multi-period production planning, the overall profit is calculated over the horizon of the whole planning periods. This chapter introduces the problem of production planning and how it is typically modelled. The opportunity to carry out integrated production is then explored. A case study is also presented to highlight the features of integrated production planning.

## ***4.2 Hierarchy of Production Planning Process***

A typical production planning process often starts with higher level decisions on the expected level of demand and prices over the planning horizon. This task is typically achieved by means of forecasting. Examples of methods for forecasting prices and demands can be found in Ye et. al. (2005) and Fouquet et. al. (1997). The forecasted information together with information on contractual orders is used in the production planning process to generate a master production schedule (MPS). MPS carries general information about the quantity of product required and when they are needed. Table 4.1 shows an example of MPS for a petrochemical plant production.

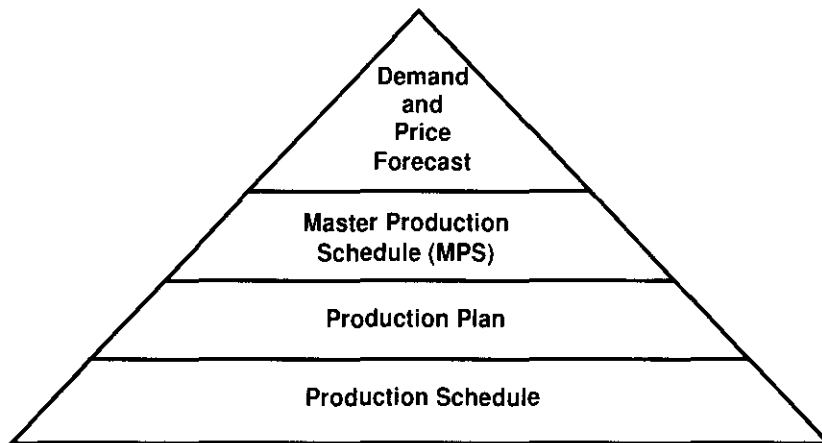
**Table 4.1: An example of MPS**

<b>Product</b>	<b>Quantity</b>	<b>Period</b>
<b>Ethylene</b>	<b>38,500</b>	<b>1</b>
<b>Propylene</b>	<b>24,500</b>	<b>1</b>
<b>Butadiene</b>	<b>8,700</b>	<b>1</b>

The MPS together with information regarding inventory status, process yields structure, and bills of lading for imported raw materials are then used to generate the production plan. The level of detail in a production plan is higher than in MPS. It typically carries information on the materials and the capacity required in order to achieve the production target.

The production planning horizon ranges from a few months to a few years. Production plan is normally proceeded by a production schedule. A production schedule provides the day-to-day information on how the plant is to be operated. Scheduling problems in the oil and petrochemical industries have been studied by Gothe-Lundgren et. al. (2002) and Tjoa et. al. (1997). Figure 4.1 summarises the hierarchy of processes involved in planning for plant production.





**Figure 4.1: Hierarchy in the Planning of Process Plant Production**

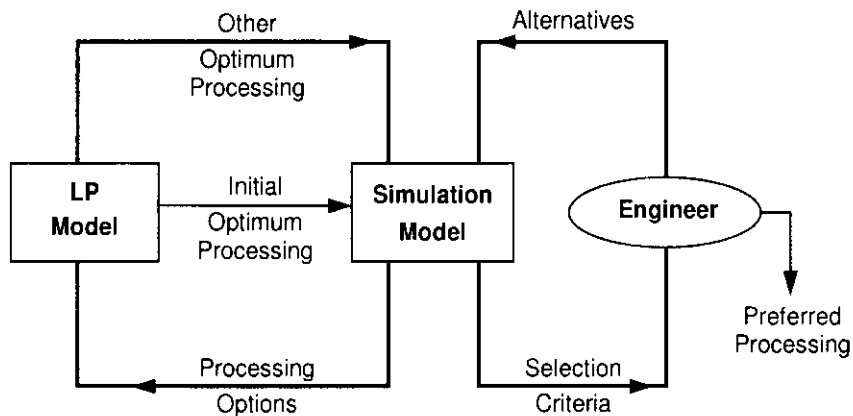
In this work, the problems of forecasting and scheduling are not investigated. The demand and prices for products as well as the prices for raw materials are assumed to be already known. These assumptions allow the problem of production planning, in particular the issue of integrated production between complimentary plants, to be explored in depth.

### ***4.3 Production Planning Models***

Formulation of a production plan can generally be classified as linear programming (LP) and non-linear programming (NLP). An LP formulation is one in which the objective function and all the constraints are linear functions. However, when a non-linear function is introduced in the objective function or any of the constraints, the production planning model becomes an NLP formulation.

LP formulation is the most common choice for production planning models. Sets of supply, demand, prices, and components are easy to build. Functions for cost, revenue and profit are formulated linearly. For multi-period production planning, planning models for individual period of production can be linked and extended to cover the whole planning horizon. Typical objective functions for the production planning optimisation problem are minimization of cost, maximization of production, or maximization of profit. However, the merit of LP formulation depends on the accuracy of technical and economic relationships at the site and the process levels. For example, by linearising highly non-linear behaviour at the process level, the linear model may lose its prediction accuracy. Poor model may lead to an overall poor LP solution.

Hartmann (1997) provides an experienced overview on the capabilities and limitations of LP formulation for planning oil refinery operations. While an LP model is capable of calculating a complete economic performance of a refinery, it is limited by the validity of the sets of linear constraints assumed in the calculation. The LP model needs to have an active interaction with a simulation model. As shown in Figure 4.2, this interaction allows the engineers to explore and test plausible scenarios through simulations. As a result, a large number of LP models are generated. These models can be solved using recursion techniques. However, the amount of computational effort used to systematically eliminate options and provide a single optimum solution is huge. Large computational efforts can be reduced by applying decomposition methods (Zhang, 2000).



**Figure 4.2: Interaction of LP model with a simulation model**

In contrast to LP formulation, an NLP formulation is able to represent the non-linear process behaviour more accurately. Non-linear process models are formulated together within the NLP model. This formulation ensures good interactions among the large number of equations used in the formulation. The effect of changes in one variable at the process level can be efficiently picked up at the site level. For example, a change in reaction temperature at the process level may result in a change of product yields. To ensure product demands are sufficiently met while keeping the profit margin at maximum, a change in feed mixture at the site-level may be imposed. Thus an NLP formulation allows the impact on economic performance to be captured more realistically.

Despite the advantages mentioned, NLP formulation suffers from the drawback of expensive problem solution. This is especially true when rigorous non-linear process models in an overall oil refinery or a petrochemical plant optimisation problem are lumped together and solved simultaneously. Solution time is lengthy as convergence is

generally slow. Furthermore, the solution can only be a global optimum solution when the objective function and the region of feasible solution are strictly convex. A convex function  $f(y)$  is defined such that when a straight line is connected between two points on the curve, then all the points on the straight line must be on or above the curve. Similarly, a convex region exists if for any two points in the region connected by a straight line and all other points on the straight line is bounded within the region (Edgar, et. al., 2001).

Much progress however has been made since the 1990's to solve NLP problems more efficiently. Viswanathan & Grossmann (1993) proposed a combined penalty function and outer-approximation method to overcome problems with non-convex NLP functions. Still and Westerlund (2005) proposed a sequential cutting plane algorithm to improve the solution speed of NLP optimisation problem. In addition to the solution methods, many applications of NLP formulations for production planning optimisation have also been reported. Moro, Zanin and Pinto (1998) developed an NLP model to optimised diesel production in an oil refinery. However, the application is limited to single period and single product problems. More recently, Neiro and Pinto (2004) used an NLP based method for the multi-period planning of petroleum supply chain. The authors also recognised the difficulty of solving large size production planning problems. Thus, they highlighted the need for a decomposition method that would solve non-linear production planning problems more efficiently.

NLP problem may also be optimised simultaneously with discrete decision variables. The resulting formulation is a mixed integer non-linear programming (MINLP) problem. In

production planning problems, the use of discrete variables may refer to the choice of feed type, operation mode, product silos, etc. Solving such a large-scale combinatorial problem with high non-convexity often leads to a very difficult problem to optimise. Depending on their structure, some problems can be solved using the decomposition approach. The outer-approximation method of Viswanathan & Grossmann (1993), for example, solves a sequence of approximate NLP sub-problem by fixing the integer variable from the master MILP problem. However, this approach can only guarantee global optimum under the condition of general convexity.

#### ***4.4 Features of Integrated Production Planning***

An example of complimentary plants is an oil refinery and a petrochemical plant. An oil refinery and a petrochemical plant produce fuel and petrochemicals for different usages. The two plants also share much of the same hydrocarbon materials within their processes. Integrated production planning aims at exploiting the production synergy that exists between these complementary plants. One way to exploit the synergy is by creating a more efficient allocation of hydrocarbon materials between the oil refinery and the petrochemical plant. The objective is to increase the profitability of both plants through optimal utilisation of their material resources.

The integrated production plan features decisions at both the site and the process levels. At the site level, firstly, oil refinery selects the optimum crude mix between two different

crude types. The crude selection is made to maximise profits of both fuel and petrochemicals production. Similarly, the petrochemical plant selects the optimum raw material mixed between high and low paraffinic contents. Secondly, the integrated production plan also decides on the best product distribution for each period. A typical example of a refinery production problem is to decide whether to operate in gasoline mode or diesel mode. Likewise, the petrochemical plant can decide whether to increase propylene production with respect to the production of ethylene during some periods or otherwise. Having different product distributions also results in different scenarios of the product inventories. Finally, the site level management also decides the level of connectivity between the oil refinery and the petrochemical plant. A simple inter-plant connectivity is easier to implement than a complex integration. However, a simple connectivity may miss an opportunity to increase profit further while complex integration may be more challenging to be implemented.

In addition to the site level decisions, the integrated production plan also features decisions at the process level. These decisions include the severity of catalytic reformer, the level of fluid catalytic cracker conversion, the coil outlet temperature of the steam cracker, etc. All of these decisions are driven by the objective of maximising the profit margins while satisfying constraints. Demands and product quality for both petrochemical and fuel products are hard constraints. These constraints must be satisfied during every production period. Other constraints are given by the process models and the physical bounds of each process unit.

The following section describes how the integrated production planning is modelled.

#### 4.4.1 Modelling Integrated Production

Options for integrated production between an oil refinery and a petrochemical plant were presented in Section 1.2. Overall formulation for production planning of individual plants has also been described in Section 3.4. This section describes modelling for integrated production strategy.

The objective during integrated production is to minimise the total production cost of the enterprise. The term “enterprise” refers to the plants that undertake the difficult task to integrate their production with the purpose of increasing their profit margin. Increase in profit margin is translated from reduction on production cost. Equation (4.1) shows the enterprise production cost,  $CT^E$  as a summation of the production costs from each of the integrated plants  $p$ . The process model constraints follow the individual plant’s

$$CT^E = \sum_p (\sum_i \sum_t c_{p,i} F_{p,i,t} + \sum_n \sum_t c_{p,n} Q_{p,n,t} + \sum_j \sum_t c_{p,j} QI_{p,j,t}) \quad (4.1)$$

constraints as per stand-alone production. However, there are additional constraints with respect to production and exchange of materials.

For integration of a final product, the following constraints are included:

- (1) For the plant supplying the final product,

$$F_{j,t} = \sum_p \alpha_{p,t} F_{p,j,t} \quad (4.2)$$

(2) For the plant receiving the final product,

$$QI_{p',j,t-1} + F_{p',j,t} + \alpha_{p',t} F_{p',j,t} - D_{p',j,t} \geq 0 \quad (4.3)$$

In Equations (4.2) and (4.3), subscript  $p$  refers to the integrated plants ( $p' \neq p''$ ).

Moreover, the term  $\alpha_{p'}$  is a variable determining the fraction of final product  $j$  from plant  $p'$  that is integrated as final product  $j$  in plant  $p''$ . It follows that  $\sum_p \alpha_p \leq 1$ .

For integration of an intermediate product, Equation (4.2) is also applicable to the plant that is supplying the product. Furthermore, the plant that is receiving the intermediate product as feed will have the following equation enforced on its capacity constraint:

$$Q_{n,p''}^L \leq \left( \sum_i F_{i,p'',t} + F_{j,p'',t} \right) \leq Q_{n,p''}^U \quad (4.4)$$

Equation (4.4) accounts for material  $j$  from plant  $p'$  that is integrated as feed  $j$  in plant  $p''$ .  $F_{j,p'',t}$  is the quantity of material  $j$  integrated during period  $t$ .

Integration of process units requires different process models because the type of feed into the process unit changes. For example, process models for the production of aromatics based on reformat and pygas feeds were discussed in Section 3.3.5. These models are also constraints in the problem formulations.



#### ***4.5 Case Study: Integrated oil refinery and petrochemical production for profit maximisation.***

This case study illustrates the features of integrated production planning. The flowsheets of an oil refinery and a petrochemical plant that were shown in Figures 3.1 and 3.3 in the previous chapter are used in this case study.

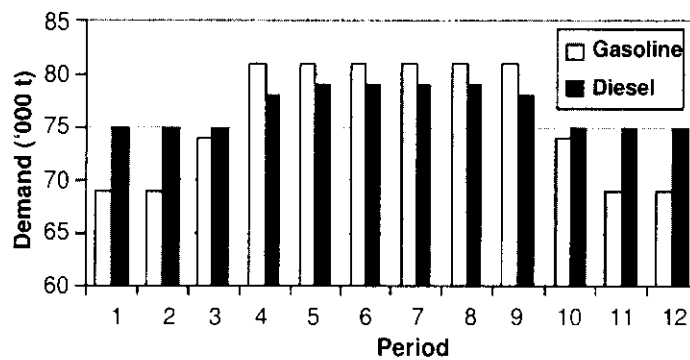
Four production options are considered. The first option (Option 1) is for both plants to maintain their stand-alone production strategy (i.e. no integration). Option 2 is for the final products of compatible chemical and physical properties to be exchanged between the two integrated plants. The third option offers intermediate products from the oil refinery as raw materials for the petrochemical plant. Finally, in Option 4, a byproduct stream from the petrochemical plant carrying valuable molecular composition can be processed using a unit in the oil refinery.

This problem involves a typical 12-month production planning period. Furthermore, the periods are assumed to be of equal length. There are two sites - the oil refinery and the petrochemical plant. The considered number of products from the oil refinery is 10 while the petrochemical plant produces 5 products. Five streams (Option 2, Option 3, and Option 4) are identified for integration. The refinery can process up to 100,000 bpd (600 t/h) of crude oil. There are two crudes to be considered for the refinery. Crude 1 is slightly lighter and sweeter than crude 2. In addition, the petrochemical plant uses multiple feed consisting of naphtha and gasoil. It can crack up to 120 t/h each of liquid naphtha and gasoil feeds. The density of gasoil is higher than naphtha but the yield of

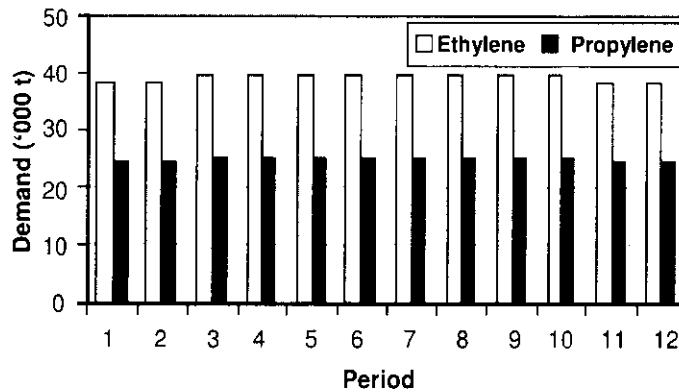
ethylene from gasoil cracking is lower. Major constraints for the oil refinery and the petrochemical plant operations are summarised in Table 4.2. Furthermore, demand constraints for some selected oil refinery and petrochemical plant products are illustrated in Figures 4.3 and 4.4 respectively.

**Table 4.2: Major constraints for oil refinery and petrochemical plant operations**

Oil Refinery Feeds		Petrochemical Plant Feeds	
Crude 1	Gravity API 34° Sulfur 1.172 wt% Cost \$125/t	Naphtha	Paraffins 69 wt% Cost \$185/t
Crude 2	Gravity API 30° Sulfur 1.244 wt% Cost \$120/t	Gasoil	Paraffins 21 wt% Cost \$150/t
Process Capacity		Process Capacity	
CDU (t/h)	min 390 to max 600	Naphtha Cracker (t/h)	min 72 to max 120
CRU (t/h)	min 72 to max 120	Gasoil Cracker (t/h)	min 72 to max 120
FCC (t/h)	min 72 to max 120	Gas Cracker (t/h)	min 6 to max 10
BTX (t/h)	min 19 to max 35		
Major Products		Major Products	
LPG, Propylene, Gasoline 95#, Gasoline 97#, Diesel, Fuel Oil, Benzene, Toluene, Xylene		Ethylene, Propylene, Butadiene, Mixed C4s, Pygas	



**Figure 4.3: Demand Constraints for Oil Refinery Production**



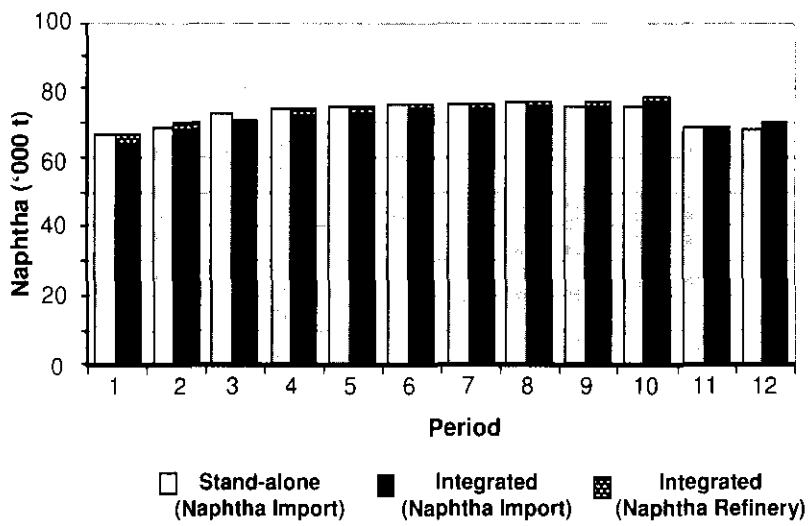
**Figure 4.4: Demand Constraints for Petrochemical Plant Production**

A non-linear programming (NLP) model for the production planning of an integrated oil refinery and a petrochemical plant is used in the case study. Key variables are operating conditions of the process units, properties of the feed streams, flowrates of feeds, flowrates of products, and flowrates of hydrocarbon materials to be integrated.

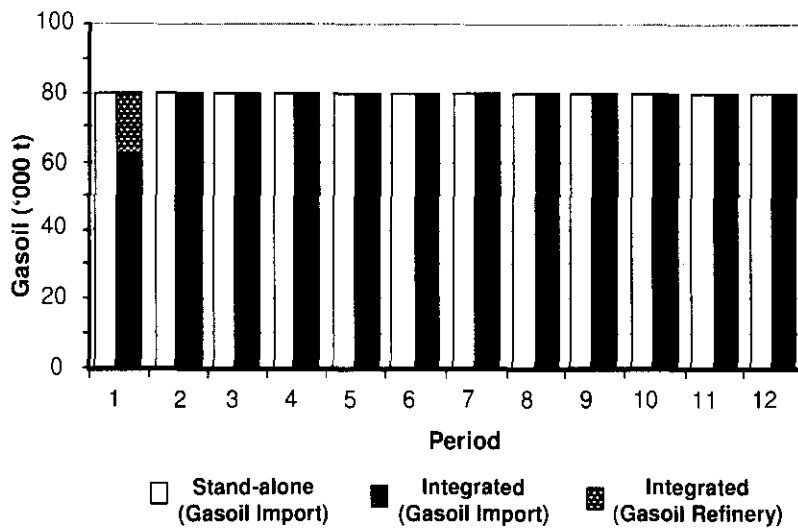
Both the oil refinery and petrochemical plant production are first optimised on stand-alone basis. Overall profit for both the oil refinery and petrochemical plants on stand-alone production are 118.35 M\$/yr and 94.67 M\$/yr respectively.

By applying the integrated production strategy, the profit increases to 125.23 M\$/yr for the oil refinery production and to 98.25 M\$/yr for the petrochemical plant production. These numbers correspond to 5.8% increase for the oil refinery and 3.8% increase for the petrochemical plant. The reason for the increase in profit is due to savings in product inventory cost. Initial inventory costs for both the petrochemical plant and the oil refinery are 4.6% and 3.2% of each of the plant's total production costs, respectively. This figure

is within the typical cost of 2.5% of total production cost reported by Shapiro (2005). When the integrated production strategy is implemented, the inventory cost for petrochemical plant drops to 1.6% of total production cost while the inventory cost for the oil refinery drops to 0.9% of total production cost. Figures 4.5 and 4.6 show the changes in petrochemical feed mix during stand-alone production and during integrated production. During the integrated production, the oil refinery shifts much of its naphtha

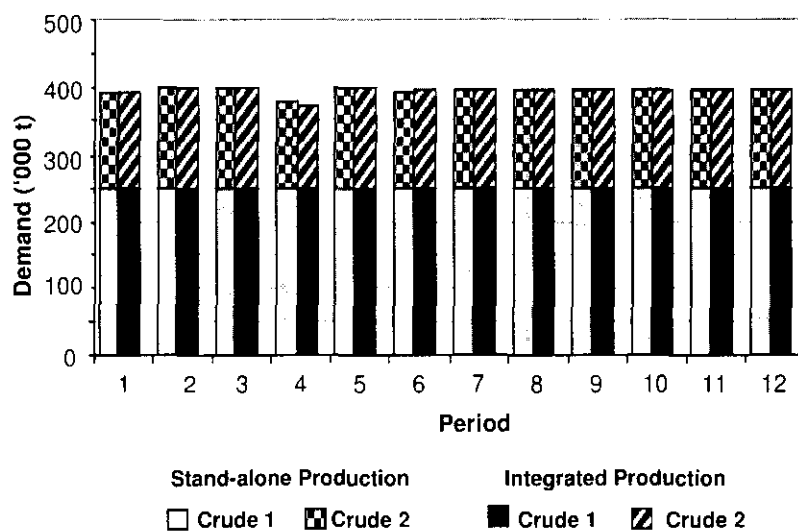


**Figure 4.5: Petrochemical's naphtha feed selection during stand-alone and integrated production.**

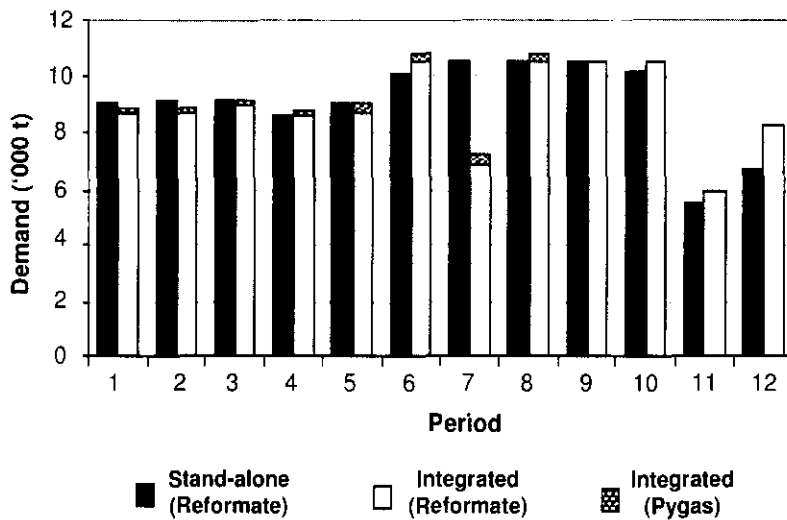


**Figure 4.6: Petrochemical's gasoil feed selection during stand-alone and integrated production.**

and gasoil inventories to the petrochemical plant. As a result, the oil refinery is able to save around 4.38 M\$/year. Furthermore, the savings is made with little effect on the optimum crude selection as shown in Figure 4.7.



**Figure 4.7: Comparison of optimum crude oil mix between stand-alone and integrated production strategies.**



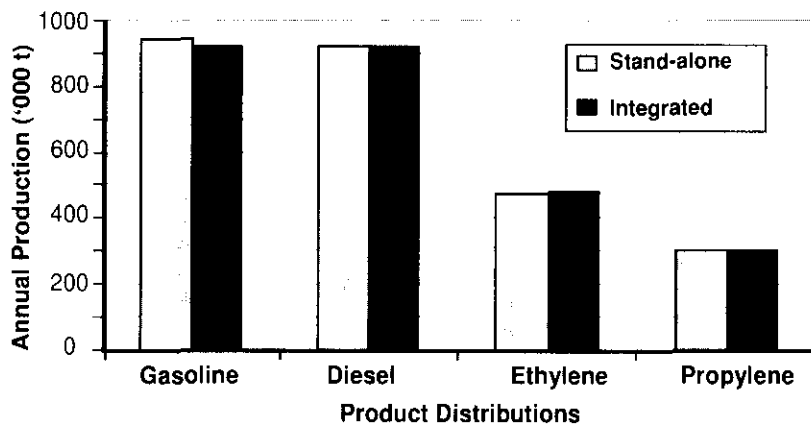
**Figure 4.8: Feed source for the production of xylene during stand-alone and integrated production.**

Similarly, the integrated production also provides an opportunity for the petrochemical plant to shift its pygas product inventory to the oil refinery. Much of the valuable benzene, toluene and xylene in the aromatic-rich pygas is extracted in the refinery's aromatic unit. Figure 4.8 compares the production of xylene during stand-alone and integrated production.

Shifting pygas inventory to the oil refinery results in nearly 65% reduction of petrochemical pygas inventory cost. The saving is huge due to the compounding effect of pygas inventory. For example, assuming the holding cost for pygas is approximately \$10 per ton per period, the strategy of integrated production is able to save the petrochemical plant about 14 M\$/yr.

Despite the huge potential for cost savings and profit improvement, this case study does not show significant impact of integrated production on the distribution of products.

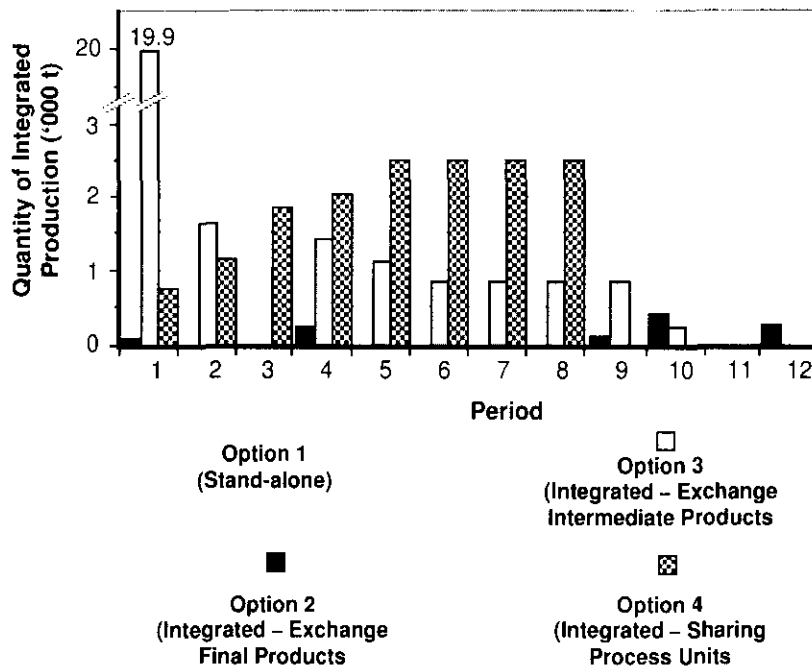
Figure 4.9 compares the distribution of major products for oil refinery and petrochemical



**Figure 4.9: Comparison of major product distributions during stand-alone and integrated production.**

plant during stand-alone and integrated production. The small reduction in gasoline production can perhaps be explained by the movement of naphtha to the petrochemical plant as feedstock. Nevertheless, the small reduction in gasoline production does not interrupt the gasoline demand and nor compromise its quality.

Process connectivity between the oil refinery and the petrochemical plant is illustrated in terms of the quantity of materials integrated during each production planning period. This is shown in Figure 4.10. The process connectivity shows that the amount of naphtha and



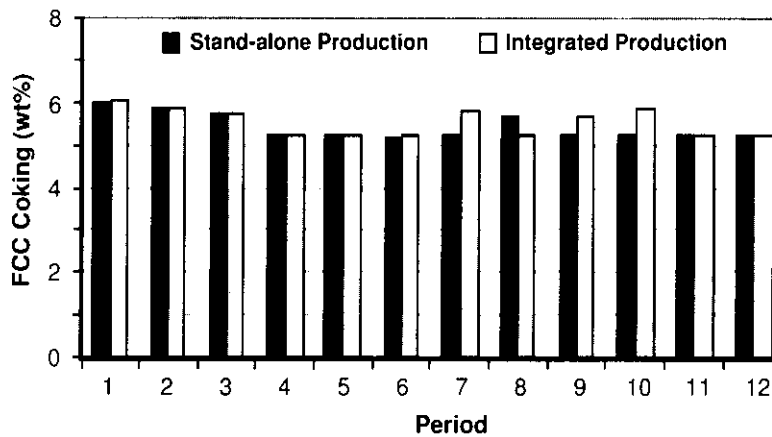
**Figure 4.10: Process connectivity between oil refinery and petrochemical plant in a multi-period integrated production plan.**

gasoil transferred from the oil refinery to the petrochemical plant is the highest in the first period. This result can perhaps be explained as a result of the oil refinery taking the steps to position the level of naphtha and gasoil inventory as early as possible during the periods of implementation of integrated production strategy. An advantage of this step is that it allows the oil refinery to concentrate on its own naphtha and gasoil demands as well as the quantity required for FCC feed and gasoline blend-stock during the rest of the production planning period. Figure 4.10 also shows that no integration is observed in period 11. The optimum production strategy for period 11 is stand-alone production. There are two reasons to explain why stand-alone production may still be an optimum choice when implementing the integrated production strategy. Firstly, it is possible that all excess inventories available for transfer have been used up in the preceding periods.



Any inventory left is only enough to satisfy the constraints until the end of the planning horizon. The second reason is due to quality difference between the integrated and the usual import materials used. For example, the usual import naphtha feed consumed by a petrochemical plant is highly paraffinic (~70% paraffin). On the other hand, the naphtha from integration with the refinery is a lower quality feedstock (~50% paraffin). Moreover, the lower quality refinery naphtha yields approximately 2% less C2-C3 olefins than the yield obtained from usual import naphtha feed. Hence the stand-alone production may be preferred. This reason is also supported by the earlier observation where large quantities of naphtha and gasoil integration occur mostly during the early periods of production planning.

In this case study, the different production strategies for the oil refinery and the petrochemical plant show no significant changes in the operating conditions of the major process units. Both the petrochemical's naphtha and gasoil crackers operate at coil outlet temperature of around 798°C and 782°C respectively. In the oil refinery, the catalytic reformer operates between a lower severity limit of RON 98 and an upper severity limit of RON 103. The FCC, furthermore, operates at around 85% conversion. The corresponding coking profiles for the FCC unit are compared in Figure 4.11 between the stand-alone and the integrated production strategy. Overall, coking of FCC during the integrated production is seen to increase by nearly 2% relative to coking during the stand-alone production strategy. Nevertheless, the choice for optimum conversion also ensures that coking is kept below an upper limit of 8 wt% while satisfying the gasoline production quantity during all production periods.



**Figure 4.11: Comparison of FCC coking profile during stand-alone and integrated production strategies.**

#### **4.6 Summary**

In production planning, decisions are made on allocation of material resources, distribution of products and operating conditions of process units. These decisions are optimised for maximum profit while satisfying all production constraints. When a synergy exists between two plants that share much of the same material, integrated production is proposed. The reason for integrated production is to exploit the flow of material resources between the two complimentary plants. In the integrated production of an oil refinery and a petrochemical plant, shifting propylene, naphtha, gasoil and pygas to the integrated plant resulted in significant reduction in product inventories. Furthermore, any changes in operating conditions of major process unit is negligible and do not upset the operations of the plant. Overall, the benefits of the integrated production strategy are

huge as it results in lower costs and higher profits to the integrated plants than in the stand-alone production strategy.

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## **Chapter 5 Strategies for Implementation of Integrated Production**

5.1 Implementation Issues.....	94
5.2 Analysis of Necessity for Integrated Production.....	95
5.2.1 Supply-Demand Pricing Model.....	96
5.2.2 Cost-Plus Pricing Model.....	98
5.2.3 Determining the Price of Exchanging Materials.....	100
5.2.4 Determining the Necessity for Integrated Production.....	104
5.3 Computational Difficulty.....	106
5.3.1 Sequential Optimisation Approach.....	108
5.4 Difficulty of Sharing Proprietary Process Models.....	110
5.5 Case Study 2: Application of New Strategies to Implement Integrated Production.....	115
5.6 Summary.....	120
5.7 References.....	121

## ***5.1 Implementation Issues***

In the previous section, despite the benefits of integrated production, three implementation issues have also been identified. Firstly, it has already been observed that stand alone production may still be an optimum strategy for some or all periods when implementing integrated production. Such a result would be costly to the plants if integration is carried out regardless of the necessity. Consequently, it becomes essential to determine whether there exists a necessity to integrate production between plants before detail work is carried out.

The second implementation issue is caused by the computational difficulty of solving non-linear models. It was observed that providing good initialisations improve the possibility for the simultaneous NLP problem to converge. However, in large NLP model such as an integrated oil refinery and petrochemical plant, there is no clear direction on what variables to initialise and what initial value to be fed. In many attempts, the engineer is only guided by experience. To overcome this difficulty, an alternative approach to programming NLP models is required.

The third issue deals with the difficulty of sharing process models. Two plants selected for integrated production are unlikely to share their process models with one another due to proprietary reason. Such barrier requires an alternative approach to getting plant's information for planning purposes without having to incorporate proprietary process models into the optimisation algorithm directly.

The following sections propose possible solutions to the implementation issues.

## ***5.2 Analysis of Necessity for Integrated Production***

In this work, sensitivity analysis is used to determine whether the benefit of integrated production is realisable as the price of exchanging materials is varied. Consider an arbitrary product from the refinery or the petrochemical plant. The revenue obtained from selling one ton of the product changes as the selling price of the product changes. Furthermore, there will be a selling price such that it is just enough to cover the minimum profit set by the company's management. In this work, this price is termed as the plant posted price (PPP).

To fully appreciate the concept of PPP, it is best to start with how typical pricing of products is carried out in the industry. Pricing is a strategic tactical issue because it positions the product in the market against rival competitors. Unless the product has technological superiority, an over-priced product will lose its market share. On the other hand, an under-price product competing for the same market share will see its profit margin reduced. This is particularly true in a globalised economy where markets all over the world tend to merge into one. There are several mechanisms used in determining the price of materials. Two of the common approaches use the supply-demand pricing model and the cost-plus pricing model (Brown, 1999; Sandholm and Suri, 2002).

### 5.2.1 Supply-Demand Pricing Model

The supply-demand model determines the price as a balance between the availability of a product at each price (supply) and the desire of those with purchasing power to purchase at each price (demand). Here, a psychological factor is involved as the price of a product often does not reflect the actual cost of producing it. Rather, it is determined by what price level buyers are willing to pay for a product at a particular time. Depending on the strength of demands for the product, the buyers usually consider the price they are willing to pay as a fair price. Figure 5.1 illustrates how the supply-demand pricing model works.

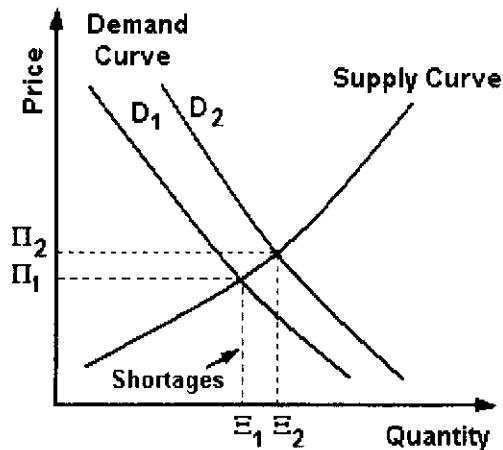


Figure 5.1: Supply-demand pricing model

The model is represented by two sets of curves: the supply curve and the demand curve. The supply curve is upward sloping while the demand curve is downward sloping. This phenomenon is not unexpected because typically when the price of a product increases, the demand naturally goes down. Likewise, higher demands are often generated when the price of a product goes down. Consequently supply and demand need to be balanced to ensure maximum revenue for the seller and minimum cost to the buyer.



Although both the demand curve and the supply curve are non-linear, they can be approximated as a linear function within a small range of quantity movement. Let the supply curve be represented by a linear function shown in Equation (5.1).

$$\pi_S = \pi_{0S} + \lambda_S \Xi \quad (5.1)$$

Similarly, let the demand curve be represented by a linear function in Equation (5.2).

$$\pi_D = \pi_{0D} - \lambda_D \Xi \quad (5.2)$$

In the above equations,  $\pi$  represents the prices at  $\Xi$  units of supply ( $S$ ) or demand ( $D$ ),  $\pi_0$  is the price at zero unit and  $\lambda$  represents the rate of change of supply price or demand price with quantity. In addition,  $\pi_{0S}, \pi_{0D} \geq 0$  and  $\lambda_S, \lambda_D \geq 0$ . There is an equilibrium price when the quantity of demand for an arbitrary product is equal to the quantity of the product being supplied. The equilibrium price occurs at an equilibrium quantity  $\Xi_{eq}$  expressed as follows,

$$\Xi_{eq} = \left( \frac{\pi_{0D} - \pi_{0S}}{\lambda_S + \lambda_D} \right) \quad (5.3)$$

Furthermore, consider an increase demand for an arbitrary product from  $\Xi_1$  to  $\Xi_2$  which disturbs the supply-demand equilibrium. From the demand curve  $D_1$ , shortages occur because the supply curve could not meet the increased demand. As shown in Figure 5.1, the demand curve must shift from  $D_1$  to  $D_2$  in order to achieve adequate supply. With the new demand curve too, there is a consequent increase in price from  $\pi_1$  to  $\pi_2$ . The new price  $\pi_2$  will bring the market-clearing point into a new equilibrium at  $\Xi_2$ . Assuming that the slope for the new demand curve is unchanged, then  $D_2$  can be found by solving Equation (5.3) for the cross-over point on the y-axis as follows,

$$\pi_{OD2} = \pi_{OS} + \Xi_2 \times (\lambda_S + \lambda_D) \quad (5.4)$$

Consequently, the new equilibrium price as demand changes from  $\Xi_1$  to  $\Xi_2$  is given by the new demand curve  $D_2$  as follows,

$$\pi_{D2} = \pi_{OD2} - \lambda_{D2} \Xi_2 \quad (5.5)$$

In the global commodity market, the prices of oil and petrochemical products are subjected to the process of bidding, selling and buying. In short, how much a buyer would pay for a barrel of crude oil or one ton of naphtha is determined from the supply-demand pricing model.

### **5.2.2 Cost-Plus Pricing Model**

Unlike the supply-demand model, the cost-plus model considers the cost of producing one ton of a product. This cost is made up of an average variable cost and an allocation of fixed cost per tonnage of product. Profit is then added as a mark-up to the total product cost. The final price of a product at the edge of its outside battery limit (OSBL) is the plant posted price (PPP). PPP can be expressed mathematically as follows,

$$PPP = \Sigma (c_{OP} + c_G) \times (1 + PR) \quad (5.6)$$

where  $c_{OP}$  and  $c_G$  are the operation cost and general expenses, respectively, in \$/t while  $PR$  is the percentage of minimum profit set by the company management. Once the product crosses over OSBL, not only will the price be subjected to psychological

supply-demand pricing, but it will also be inflated due to numerous governmental taxes applied on it. The type of taxes incurred varies with the location of the plant. Some examples of taxes are municipal taxes, state taxes, value added taxes and environmental taxes.

Operation cost consists of fixed cost,  $c_F$ , and variable cost,  $c_V$ , as shown in Equation (5.7). Fixed costs are charges typically unaffected by the rate of plant production.

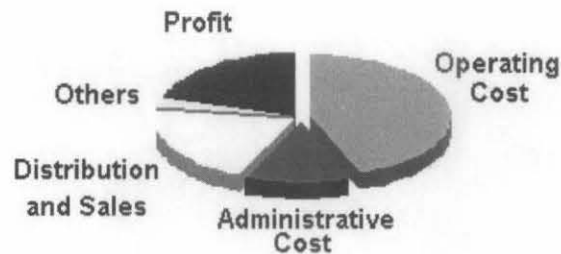
$$c_{op} = \sum (c_V + c_F) \quad (5.7)$$

Examples of this cost include site rentals, insurance and property taxes. On the other hand, variable costs are expenses that vary with the plant throughput. Variable cost can be grouped into direct cost,  $c_{V,direct}$ , which is directly related to plant operations and indirect costs,  $c_{V,indirect}$ , as shown in Equation (5.8). General expenses are an indirect

$$c_V = \sum (c_{V,direct} + c_{V,indirect}) \quad (5.8)$$

cost because they are not directly related to plant operations. Examples of general expenses are administrative cost, distribution and sales cost, and other minor costs such as interest paid on financing. Direct operation costs are made up of production costs and plant overhead costs. Fixed cost is a non-variable component of direct operation cost. Production cost involves expenditures for raw materials and costs related to raw materials transportation, unloading and storage. Production costs also include operating labours, utility costs, plant maintenance, operating supplies, catalysts, process licensing fee, and many more. Plant overhead costs cover the general maintenance overhead, safety and

security services as well as expenses for medical and hospitalization. Figure 5.2 below shows a typical composition of PPP based on the cost-plus pricing model.



**Figure 5.2: A typical cost-plus pricing model to determine PPP**

### ***5.2.3 Determining the Price of Exchanging Materials***

Supply-demand pricing is used to determine the price of a product where competition exists between buyers and sellers world-wide. In the case of integrated production, competition for exchanging materials between the integrated plants does not exist. The plants decide to integrate on mutual understanding that the strategy will bring benefit to both plants through shifting of excess product inventory. For this reason, PPP based on cost-plus pricing model is selected as the basis to determining the price of exchanging materials.

Consider the task of determining the price of refinery naphtha to be integrated with a petrochemical plant. Direct cost for producing one ton of naphtha from crude oil is calculated based on naphtha yields averaged over a 12-month period. Similarly, other cost are also calculated based on plant's historical yield information, typically as a fraction of product cost or plant's capacity. Operating labour cost is estimated for a

strongly automated plant. Other costs that made up the operation cost and general expenses are estimated as a factor of plant capacity or total product cost. Guides to some typical correlations are also published in the literature (Peters et. al, 2003; US Department of Energy, 2003). Table 5.1 shows how the cost-plus model is used to arrive at the plant posted price (PPP) as per Equation (5.6).

**Table 5.1: Calculation of naphtha’s plant posted price (PPP)**

Price per ton of naphtha	(\$/t)
Direct material cost	6.35
Direct Operating Labour	3.40
Supervisory & Clerical Labour	0.85
Utilities	1.52
Maintenance	0.14
Operating Supplies	0.01
Laboratory Charges	0.17
Licensing Fees	1.58
Total Direct Cost	14.03
Fixed Charge	30.20
Plant Overhead	23.70
<b>Operating Cost</b>	67.93
<b>Administration</b>	18.96
<b>Distribution and Sales</b>	31.60
<b>Other Expenses</b>	3.95
<b>Total Product Cost</b>	122.44
<b>Profit</b>	30.61
<b>Plant Posted Price (PPP)</b>	<b>153.04</b>

The price of exchanging materials must be lower than the market price for the integration of materials to be profitable. The price should therefore be determined from the value the integrated material has on both plants. The concept of netback is used to determine this

value (Julka, N. et. al., 2002). Netback is the value of a material based on the profit it generates. The pre-logistic netback value can be expressed as,

$$\text{Netback} = \sum x_j c_j - c_M \quad (5.9)$$

where  $x_j$  is the yield of product  $j$ ,  $c_j$  is the unit price of product  $j$ , and  $c_M$  is the cost per ton of raw materials. The final netback value takes into account the logistical cost of product storage and distribution.

For the integration of refinery material – for example, naphtha - with a petrochemical plant, netback is used to evaluate the value of naphtha as follows:

- (1) To Oil Refinery: The contribution of naphtha sales to refinery profits plus the savings it makes from reduced naphtha inventory.
- (2) To Petrochemical Plant: The sales price of naphtha cracking products minus the cost incurred in purchasing, processing and distributing the products.

Table 5.2 summarises an example of how the netback is calculated for both the refinery and the petrochemical plant. In this example, the minimum profit was assumed at 20%.

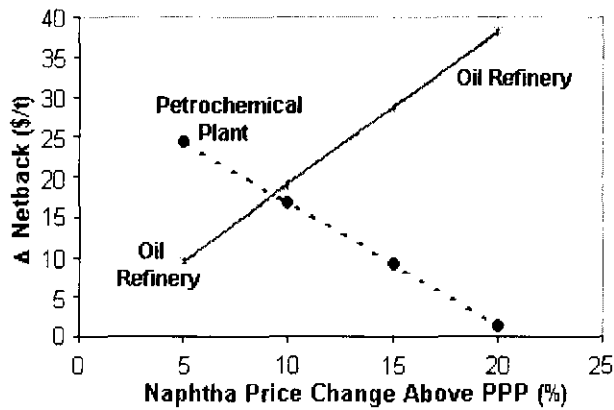
The price of naphtha is varied with respect to the plant posted price between PPP and 20% above PPP. The netback at each naphtha price is then recorded. The variation of oil refinery's and petrochemical plant's netback with respect to changing naphtha price is shown in Figure 5.3. It is observed that as the price of naphtha is increased above PPP,

the oil refinery gains a positive netback change. However, for the same increase in naphtha price, the petrochemical plant incurs a negative netback change.

**Table 5.2: Calculation of refinery and petrochemical netback**

<b><u>Refinery Netback Calculations</u></b>		
	Yield (t/t)	Contribution (\$/t)
<b>Fuel</b>	0.7144	117.01
<b>Intermediates</b>		
Naphtha	0.0516	9.28
Gasoil	0.0810	11.75
Residue	0.1033	10.84
<b>Olefin</b>	0.0046	1.77
<b>Aromatic</b>	0.0448	13.55
	SubTotal	164.21
Less	Materials	123.17
	Distribution & Storage	7.00
	<b>Netback (\$/t)</b>	<b>34.04</b>

<b><u>Petrochemical Netback Calculations</u></b>		
	Yield (t/t)	Contribution (\$/t)
<b>Olefins</b>	0.5325	208.63
<b>Intermediate</b>	0.2479	37.18
<b>Fuel</b>	0.2198	6.55
	SubTotal	252.37
Less	Materials	171.93
	Distribution & Storage	7.00
	<b>Netback (\$/t)</b>	<b>73.44</b>



**Figure 5.3: Effect of naphtha price change on the change of netback for oil refinery and petrochemical plant**

While it is the prerogative of the management of both integrated plants to agree on the price of exchanging materials, the method shown above highlighted one possible price that is about 9.3% above PPP. This price is a win-win price since the refinery can still make reasonable profit, while the petrochemical plant can get a cheaper feed material. For the market price of naphtha at \$180/t, the suggested exchanging material price is \$167.22/t or approximately 7.1% lower than the market price.

#### **5.2.4 Determining the Necessity for Integrated Production**

PPP is the price of the product at the edge of the plant's outside battery limit (OSBL). Once the product crosses over OSBL, the selling price could go higher than PPP or go lower than PPP. This is because once the product is outside OSBL, in addition to the various taxes incurred, the direction for the selling price of the product is driven by market forces. If the market selling price matches the PPP, then the plant achieves minimum profit for the product. Moreover, the plant can achieve higher than minimum



profit if the market price is higher than PPP. However, if the market price is lower than PPP, the plant will not only achieve lower than minimum profit but it is also possible that the plant will be selling the product with losses.

**Table 5.3: Sensitivity analysis to determine the necessity for integration**

Refinery Naphtha Price	Refinery Profit Change	Petrochemical Profit Change	
Naphtha Price above PPP	Positive Profit Change	Negative Profit Change	} Refinery Gain, Petrochemical Loss
PPP	Zero	Zero	
Naphtha Price below PPP	Negative Profit Change	Positive Profit Change	} Petrochemical Gain, Refinery Loss

↑  
 Win-Win  
 ↓

Consider again the integration of refinery naphtha with a petrochemical plant. Table 5.3 shows the sensitivity analysis to determine how the selling price of naphtha determines the necessity to integrate refinery's naphtha with the petrochemical plant. If the price of naphtha is sold at any price lower than PPP, the refinery will incur profit losses while the petrochemical plant will gain profit. In addition, should the selling price of refinery naphtha be higher than PPP, then the petrochemical plant will incur huge profit losses while the refinery will gain profit increase. However, the sensitivity analysis also shows that there is a band (shaded area) of refinery naphtha selling price between PPP and up to some price higher than PPP, where an opportunity exists for both the refinery and the petrochemical plant to gain increase profits through integrated production. Increased

petrochemical profit is due to lower cost of feeds. Increase for refinery profit is not only due to higher product price but also to reduced cost of naphtha inventory. As a result, the necessity for integration can be determined through sensitivity analysis. Determining the necessity for integration at an early stage of the project also helps to rule out unnecessary work at a later stage.

### **5.3 Computational Difficulty**

In executing simultaneous optimisation of multi-period production planning, a problem was often encountered with respect to the initial value for the calculation to take place. In default, the initial point for all variables for which the values are unknown is zero. This then creates computational problems especially when the initialised variables are used as denominators in some equations.

In many equations, problems encountered with division by zero can be avoided by re-expressing the form of an algebraic equation. For example, consider equation 5.10 shown below. In this equation, both  $y_1(i)$  and  $y_2(i)$  are declared as positive variables.

$$y_1(i) = \frac{1}{y_2(i)} \quad (5.10)$$

The equation will create a computational problem on the right hand side of the equation if an initial value is not provided to  $y_2(i)$ . Hence the default value used by the

computation for  $y_2(i)$  is zero. Consequently the computation can not proceed with the next iteration because of a division by zero error.

Equation (5.10) can be rearranged by bringing both variables onto the left hand side of the equation. As shown in equation (5.11), even if the variables are not initialised, the computation can still proceed into the next iteration. The simple illustration shows that simple re-expression of equations can help provide a stable computation output.

$$y_1(i) \times y_2(i) - 1 = 0 \quad (5.11)$$

In the production planning problem, a default zero initial value also creates a feasibility problem. The problem arises when an equation requires input variables that are only calculated at some point further down in the program. For example, the production of gasoline depends on the value of feed quantity into the crude distillation unit. This value has a lower bound of zero and an upper bound equal to the capacity of the refinery. For a minimisation problem, since the feed adds cost to the production, the computation will start with a default value at the minimum bound of the feed flow rate. Due to the zero feed value, all other calculations that depend on feed – for example feed to reformer – will be zero. As a result, infeasibility occurs because even though the objective function of finding a minimum cost function is reached, the constraints of meeting the demand are not achieved.

Computational problems encountered with respect to initial values can usually be overcome by assigning an initial value for some of the variables. However, during the

programming stage, because of the large number of variables involved, it is often not clear which of the large number of variables require initialisation. Moreover, initialisation of variables is difficult because it may lead to poor convergence. An engineer is often guided only by experience that comes after numerous trials-and-errors. In the end, the number of initialisation is often large.

In this work, a new approach is proposed to avoid the problem of supplying large number of initial values. Rather than lumping all the models and solving them simultaneously, the proposed approach is to build and optimise the models sequentially. The sequential optimisation approach is discussed in the following section.

### ***5.3.1 Sequential Optimisation Approach***

The sequential modular approach has been popular against the equation-oriented approach in flowsheet simulation task. The idea is to model and simulate one unit operation at a time. Problem encountered during modelling can be specifically located and rectified immediately.

The sequential flowsheeting approach usually starts from the front-end unit operations where most of the variables are already known. Recycles can be handled fairly easily using tearing technique. In this technique, unknown values, for example recycle flowrates, are initially assumed as closed to the expected values. The model is then iterated until a converged value is achieved.

The difference between sequential simulation and sequential optimisation lies in the number of degrees of freedom. In a simulation problem, the number of variables is matched by the number of equations. This results in a zero degree of freedom. However, in an optimisation problem, there can be more variables than there are equations. The degree of freedom is therefore positive and at least one of the variables can usually be optimised (Edgar, et. al., 2001).

The sequential approach also avoids solving large models. Smaller models in the sequential approach make the algorithm easier to be understood and to be solved. Any logic problem can easily be traced to each model. This greatly aids the debugging stage. Furthermore, any additional features to improve the program can be easily included. For example, operation engineers may want to include a model that is only unique to specific process into the formulation. Likewise, changes in future operational practice may require the formulation to be modified or expanded. These features can be performed on the individual model itself or by creating a new model to perform specific functions. Thus, the ease in modelling sequentially also helps in lowering the cost of solving large production planning optimisation problems.

Figure 5.4 illustrates the concept of the sequential optimisation technique. During the first iteration level, only a small number of initial values are provided. Each process model is solved sequentially. The solution from a process model is used by other process model down in the flowsheet. The generation of individual solutions provides the input for the

calculation of overall cost model and to the overall objective of optimisation. During each iteration stage, the objective is compared to the previous objective. The iteration continues until no more improvement in the objective value is possible.

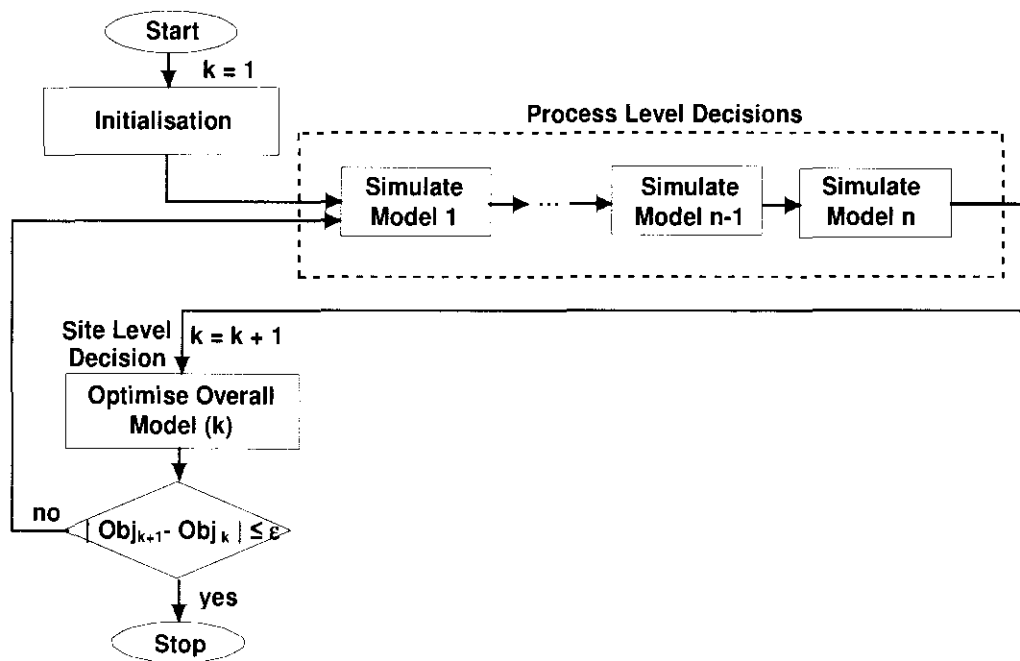


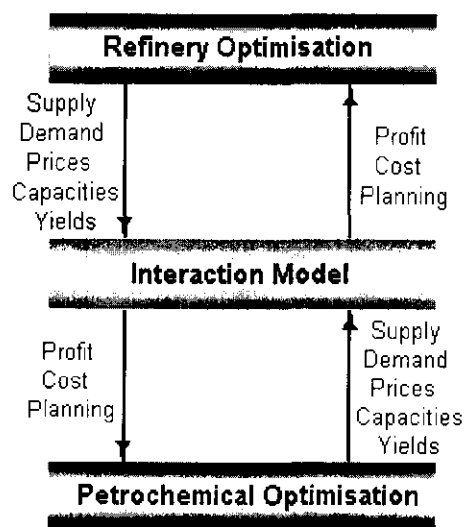
Figure 5.4: Sequential optimisation approach

### 5.4 Difficulty of Sharing Proprietary Process Models

The ability to predict yields as the quality of feed and the operating conditions of the plant change is paramount to generating an optimum production plan. This prediction is generated from plant's process model. However, it is unlikely for two different plants to

share their proprietary process models. This barrier prevents all models from being lumped together and solved simultaneously. Nevertheless, the modularity of the sequential optimisation approach makes it possible to implement integrated production without having to share process models with the other plant. The approach adopted in this work is to build an interaction model that bridges the information between the two plants. In this way, information generated from process models in one plant can interact with information from another plant without having to access the models themselves.

The role of the interaction model is to regulate what information is required from both plants. This information provides the vital input for optimisation of integrated production planning. The interaction model also screen which integration option to be selected for both plants during each planning period. For example, consider the integration of refinery naphtha with a petrochemical plant. The objective for each plant is to minimise its' total cost of production as per Equation (3.15). The optimum objective value for the stand-



**Figure 5.5: Interaction model**

alone plant along with information on supply, demand, prices, capacities and process yields is then passed to the interaction model. The interaction model uses this information along with possible integration options to find an improved solution.

An improved solution is searched through the different options available for integrated production as discussed in Section 1.2 previously. Each option generates a network between the refinery flowsheet and the petrochemical plant flowsheet. The architecture of the network is generalised in Figure 5.5. For naphtha integration, the interaction model requires the following information from each plant:

- Refinery crude supply,  
 $FCrude(n)$ , for all  $n$ .
- Refinery naphtha yield,  
 $CrudeTBP(yield, naphtha)$ .
- Refinery naphtha demand,  
 $DemandRef(n, naphtha)$  for all  $n$ .
- Petrochemical supply of imported naphtha,  
 $FNaphthaIm(m)$  for all  $m$ .
- Petrochemical steam cracker yield on imported naphtha  
 $xImSCN(k, m)$  for all  $k, m$ .
- Petrochemical steam cracker yield on refinery naphtha  
 $xRSCN(k, m)$  for all  $k, m$ .
- Petrochemical product demand  
 $DemandPCh(k, m)$  for all  $k, m$ .

In the above list, index  $k$  refers to a set of petrochemical products while indices  $n$  and  $m$  are sets of production period for the refinery and petrochemical plant, respectively. Based on the integrated production network generated, the interaction model incorporates a multiplier  $\alpha$  on the flow of refinery naphtha stream allocated for the petrochemical plant.



The flow of each product stream is controlled by the individual plant as per Equation (5.12). However the multiplier  $\alpha$  adds an additional mass balance constraint to the refinery as follows:

$$\left. \begin{aligned} F_{j,t} &= \sum_p (\alpha_{p,t} F_{p,j,t}) \\ \sum_p \alpha_{p,t} &\leq 1 \end{aligned} \right\} \forall p,t \quad (5.12)$$

The multiplier  $\alpha$  is a variable decided by the interaction model. It acts to optimise the production of naphtha in the refinery and the consumption of naphtha in the petrochemical plant. For each feasible value of  $\alpha$ , the individual plant calculates the total cost as per Equation (3.15). Other constraints are on the capacity of petrochemical plant,

$$Q_{n,p'}^L \leq \left( \sum_j F_{i,p',t} + F_{j,p',t} \right) \leq Q_{n,p'}^U \quad (4.4)$$

and on the inventory level of refinery naphtha,

$$\left. \begin{aligned} QI_{j,t-1} + (1 - \alpha_t) \times F_{j,t} - D_{j,t} &\geq 0 \\ \alpha_t &\leq 1 \end{aligned} \right\} \forall t \quad (5.13)$$

Revenue and profit at each feasible value of  $\alpha$  are calculated by individual plant as per Equations (3.1) and (3.16) respectively. The total enterprise cost as per Equation (4.1) is calculated by the interaction model and compared with the combined costs of stand-alone production. If the interaction model finds a solution that is better than the existing plants' stand-alone solution, then profit, cost and new optimum planning information are then returned to the individual plant. Where integration occurs, the interaction model would provide the individual plant on what material to integrate, the quantity to integrate and the period where integration is to be implemented.

convergence criteria,  $\epsilon$ , the procedure then returns the optimum production planning information to the individual plants and stops. Otherwise, the search for other options of integrated production network continues.

### ***5.5 Case Study: Application of New Strategies to Implement Integrated Production***

The purpose of this case study is to apply the three strategies developed in Sections 5.2, 5.3, and 5.4 in the implementation of integrated production. A simple problem involving options for propylene integration between an oil refinery and a petrochemical plant is selected. Both the oil refinery and the petrochemical plant produce propylene from FCC unit and the steam cracker units respectively. Propylene integration is simple because it only involves the exchange of final products. The quantity of propylene available for integration is also small due to the small demand of refinery propylene. Nevertheless, this case study should be sufficient to demonstrate the application of the new implementation strategies developed in this chapter.

Firstly, sensitivity analysis is used to explore if propylene integration will bring benefit to both the refinery and petrochemical plant. The market selling price for propylene is assumed at \$400/t over the whole planning horizon. PPP is then calculated as per Equation (5.6). Assuming an arbitrary value of minimum profit at 30%, the PPP for refinery propylene is approximately \$165/t.

Consider an oil refinery selling its' excess propylene product in inventory to a petrochemical plant. For every ton of propylene produced by the refinery, the contribution to profit by the quantity of propylene sold to the petrochemical plant can be calculated as follows:

$$\begin{matrix} \textit{Profit} \\ \textit{Contribution} \\ \textit{Refinery} \end{matrix} = \alpha_j \times F_{p,j} \times (\pi_j - c_j) \quad (5.14)$$

In Equation (5.14), index  $j$  refers to propylene product and index  $p$  the refinery. Then,  $\alpha_j \times F_{p,j}$  is the quantity of refinery propylene sold to the petrochemical plant under the strategy of integrated production,  $\pi_j$  is the unit price of the exchanged material, and  $c_j$  is the unit production cost for the oil refinery. Furthermore, the contribution of refinery propylene to the profit made by the petrochemical plant can be calculated from Equation (5.15). Assuming the quality of refinery propylene product is identical to the quality of

$$\begin{matrix} \textit{Profit} \\ \textit{Contribution} \\ \textit{Petrochemical} \end{matrix} = \alpha_j F_{p,j} \times (\pi^*_j - \pi_j) \quad (5.15)$$

petrochemical propylene product, then the only cost incurred by the petrochemical plant is the purchase cost  $\pi_j$ . With this assumption, the petrochemical plant can make a clean profit by selling the refinery propylene at the market price  $\pi^*_j$ .

Table 5.4 shows the sensitivity analysis for refinery propylene integrated with the petrochemical plant. The selling price of refinery propylene to the petrochemical plant is varied in the range of  $\pm 20\%$  from the PPP. Profit is calculated per ton of propylene exchange. If the refinery propylene is sold at PPP, then the refinery makes no change in

profit. Likewise, if the petrochemical plant purchases the refinery propylene at the market price, then the petrochemical plant gains no benefit from the integrated production strategy. It is only when the price of refinery propylene goes below its' market price, then the petrochemical plant will see huge benefit of integrated production. The huge benefit is caused by the large difference between refinery PPP and the market price for propylene. However, the refinery will unfortunately see a negative profit change if its' propylene is sold to the petrochemical plant at a price below the PPP. Table 5.4 also shows that there is a region between the PPP and the market price whereby both the oil

**Table 5.4: Sensitivity analysis to determine the necessity for propylene integration**

<b>Refinery Propylene Price</b>	<b>Refinery Profit Change</b>	<b>Petrochemical Profit Change</b>
<b>Market Price</b>	<b>675 %</b>	<b>Zero</b>
<b>20% above PPP</b>	<b>95%</b>	<b>405 %</b>
<b>10% above PPP</b>	<b>47 %</b>	<b>446 %</b>
<b>PPP</b>	<b>Zero</b>	<b>487 %</b>
<b>10% below PPP</b>	<b>-47%</b>	<b>529 %</b>
<b>20% below PPP</b>	<b>-95 %</b>	<b>570 %</b>

} win-win

refinery and the petrochemical plant have the potential to benefit from integrated production strategy. Consequently, the necessity for propylene integration between the oil refinery and the petrochemical plant has been determined.

Having determined the necessity for propylene integration, the integrated production between the oil refinery and the petrochemical plant is implemented using the sequential optimisation approach. The objective function is minimisation of total enterprise cost as per Equation (4.1). The solution generated by sequential optimisation approach is compared to the solution generated from simultaneous optimisation for the same case study. As shown in Table 5.5, the objective values reached by both approaches differ only by about 1.5%. The small magnitude of the difference perhaps points to cause of the difference being propagated from the numbers in the calculation itself.

**Table 5.5: Comparison of performance between simultaneous and sequential optimisation approach**

	<b>Simultaneous Optimisation</b>	<b>Sequential Optimisation</b>
<b>Objective Value ('000 \$)</b>	973,720	987,982
<b>Number of Variables</b>	3,038	3,308
<b>Number of Initialisations</b>	161	18
<b>Iteration Count</b>	> 100,000	25,562
<b>Resource Usage (s)</b>	376	72

In terms of computational performance, the sequential optimisation approach uses more variables than the simultaneous optimisation approach. The higher number of variables is caused by the higher number of models to be optimised sequentially. In spite of this, the sequential approach requires much less initialisation than the simultaneous approach.

This attribute is very helpful as it meant that the sequential optimisation approach is more user friendly.

The computations are run on a Window XP operating system supported by Pentium 4 microprocessor at 3 GHz speed and 512 MB memory. The number of iterations encountered during simultaneous optimisation is more than 4 times higher than the number of iterations encountered by the sequential optimisation approach. In addition, the resource usage by simultaneous optimisation approach is 5 times higher than the usage by sequential approach. Resource usage refers to the CPU time required by the solver. As a result, the solution generated by the sequential optimisation approach is more efficient than the solution generated from the simultaneous optimisation approach.

Finally, the modularity of the sequential optimisation approach also allows for a third party interaction model to be easily incorporated into the implementation procedure.

Overall, this case study has highlighted that the performance of sequential optimisation approach is superior to the performance of simultaneous optimisation approach.

## **5.6 Summary**

This chapter discusses the implementation issues encountered in the previous approach. New implementation strategies are proposed. The necessity to integrate is first determined at an early stage before performing detail implementation tasks. Detail implementation tasks include generating options of integrated production network. The generation of options requires building individual process models and overall cost models. Sequential optimisation approach is proposed for this task. Moreover, the modularity of the approach enables a third party interaction model to be easily incorporated. The interaction model ensures that the integrated plants do not have to compromise their proprietary process models. Furthermore, the pricing mechanism used in determining the price of exchanging materials is based on the cost-plus approach. A case study is presented to demonstrate the application of the new implementation strategies. The performance of the sequential optimisation approach has shown better solution efficiency than the previous simultaneous optimisation approach.

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## ***Chapter 6 Uncertainty and Flexibility***

6.1 Introduction.....	123
6.2 Uncertainty in Demand and Prices.....	124
6.3 Quantifying Uncertainty.....	126
6.3.1 An Example for Quantifying Uncertainty.....	129
6.4 Solution Approaches to Problems with Uncertainty.....	131
6.4.1 An Example of Production Planning under Uncertainty.....	133
6.5 Feasibility Analysis of Integrated Production Planning under Uncertainty...	134
6.6 Case Study 3: Flexible Integrated Production under Uncertain Demand and Prices.....	137
6.7 Summary.....	145
6.8 References.....	146

## **6.1 Introduction**

A global market is filled with volatility. Customer expectations are constantly changing and many uncertainties exist. There are various sources for uncertainty - rushed or cancelled orders, equipment failure, plant shut-down, opening of new markets, seasonal change in demand, price fluctuations, and many more.

The analysis on an integrated production strategy has so far been performed on prices and demand that are assumed to be known with certainty. However, except for contractual arrangements made for raw material supply and product demand, demand and prices are subject to uncertainty in the future. Consequently, it is difficult to say if a production plan produced under assumptions of fixed demand and prices is still useful should the demand or prices of some materials changes during some period in the future. Failure to account for uncertainty in demand and prices reduces the flexibility of the production plan. On one extreme, the survivability of the company may be threatened. On the other extreme, the company might miss an opportunity to take advantage of a profitable market environment. Swaney and Grossmann (1985) defined a flexible system as one that continues to be feasible under a range of uncertain parameters. Hence, for a production plan to be flexible, it must be feasible throughout a range of uncertainty, for example, in demand and prices.

This chapter analyses the issue of flexibility and uncertainty in planning for integrated production. Steps to assure feasible operations under uncertainty are also suggested.

## **6.2 Uncertainty in Demand and Prices**

Demand and prices for an oil refinery's and a petrochemical plant's products are affected by the market forces as well as by the political forces. Figures 6.1 and 6.2 show a 60-month historical price ratio of naphtha and gasoil to the price of crude oil (Ratio P/F). Furthermore, the plots are superimposed on a 60-months historical demand for naphtha and gasoil for the same period. Data for the historical demand and prices are collected from the Oil and Gas Journal<sup>‡</sup> for the period between January 1990 and December 1994.

Two distinct behaviours can be observed from the plots. Firstly, trends of demand and price ratios seem to repeat themselves in a cycle. This reflects the seasonal demand and price change of these materials in an equilibrium market and a peaceful political environment. Secondly, however, the harmonious cycle can be interrupted by a sudden increase in demand and prices. These are observed as spikes within the cyclical trends. One possible reason for these spikes is perhaps caused by a troubled political environment such as a war. Another reason for these spikes is the opening of a new market. A new market often disrupts the market equilibrium by heavy demand that exceeds current supply.

It is concluded from these two plots that it is possible to forecast the price and demand of fuel and petrochemical products based on experience of the past. However, the uncertainty of the two parameters cannot be totally eliminated due to unknown political and market situations in the future.

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<sup>‡</sup> Oil and Gas Journal , PennWell Corp., 1421 S. Sheridan Rd., Tulsa, OK 74101-1260, USA.

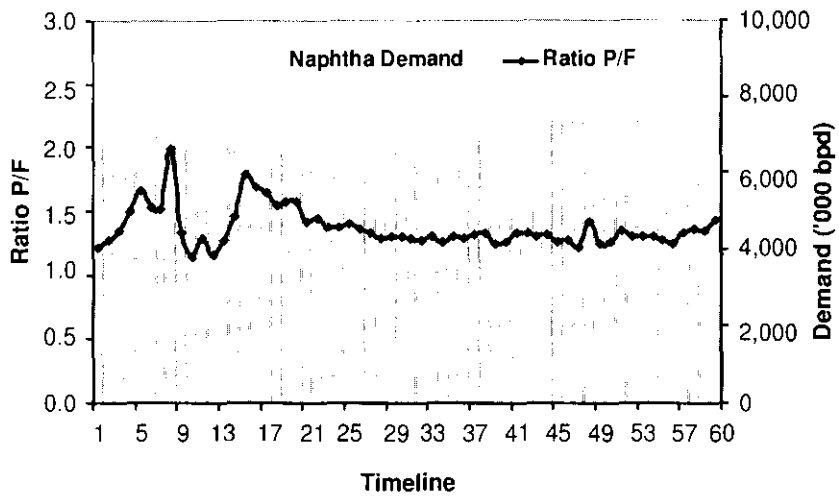


Figure 6.1: Historical profile of uncertainty in naphtha demand and price

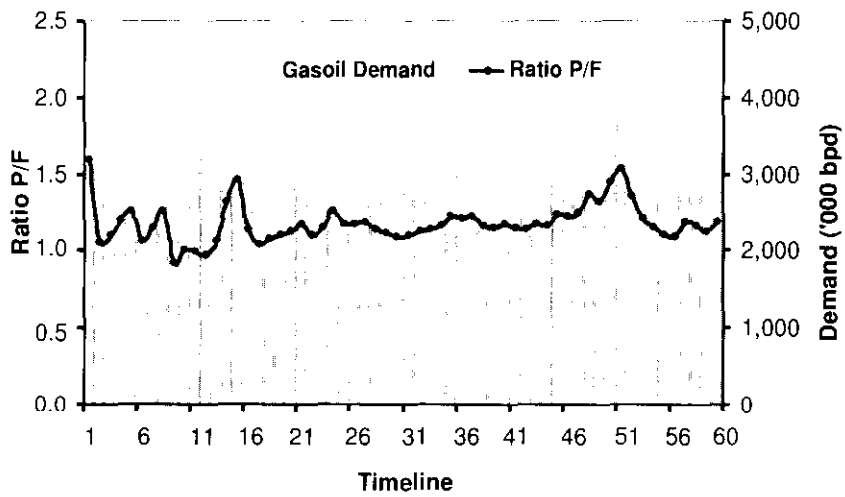


Figure 6.2: Historical profile of uncertainty in gasoil demand and price

### 6.3 Quantifying Uncertainty

Uncertainty in demand and prices cannot be ignored. For an integrated production plan to be flexible, it has to remain feasible even when these parameters vary. Variations in the demand and price data are enumerated in terms of the average values, the range of the historical data, and the standard deviations.

The average is the most commonly used measurement to describe how the data are distributed. In a normal distribution curve, the average would point to the centre of the distribution. Mathematically, the average of a set of values  $y$  is defined as

$$\bar{y} = \frac{\sum y}{n} \quad (6.1)$$

where  $\bar{y}$  is the average value and  $n$  is the total number of values. For example, the average of naphtha price in the 60-month period ( $n = 60$ ) as shown in Figure 6.1 is 195.16 \$/t.

While the average points to the centre of the distribution, the spread of the distribution can be measured by the range and the standard deviation. The range is a simple measurement of variability. It measures the difference between two extreme values (i.e. the highest and the lowest values) in a distribution. For example, the price range of naphtha as per Figure 6.1 is 196.58 \$/t. The magnitude of the range is more than 50% of the minimum price of naphtha at 128.50 \$/t. Consequently, the range shows that the spread of naphtha price for the 60-month period is acceptably wide. The standard deviation is a measure of the variability of the data. Variability shows the degree to which

a value  $y$  deviates from the average value  $\bar{y}$  in a distribution. Equation (6.2) shows how a standard deviation  $\sigma$  is calculated:

$$\sigma = \frac{\sum (y - \bar{y})^2}{n - 1} \quad (6.2)$$

Hence, the standard deviation for the 60-month historical price of naphtha is 42.92 \$/t.

Consider one standard deviation or  $1\sigma$ . At  $1\sigma$ , the price of naphtha has the probability to vary by 22% from a given price. In statistical control practice, an upper limit is usually set at  $3\sigma$  above an average. Similarly, the lower limit is set at  $3\sigma$  below an average. By plotting the demand and price movement within  $\pm 3\sigma$ , an x-bar chart histogram can then be constructed. The x-bar chart quantifies the probability for uncertainty of a given parameter. In addition, the r-charts shows the parameter within variations within  $\pm 3\sigma$ . Figures 6.3 and 6.4 show the x-bar chart along with the r-chart for price and demand uncertainty of naphtha. The modal for price uncertainty falls within  $-1\sigma$  while the modal for demand uncertainty falls within  $+1\sigma$ .

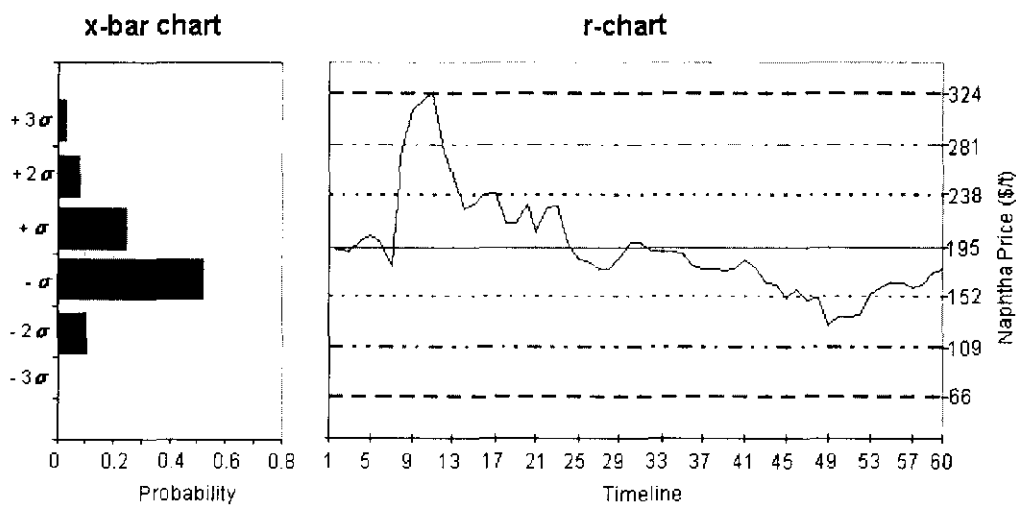
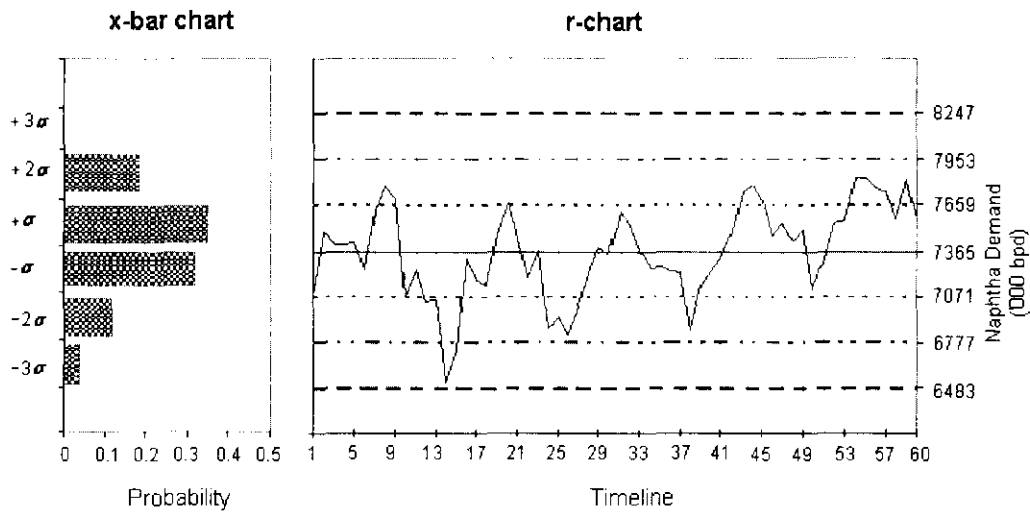


Figure 6.3: Quantifying naphtha price uncertainty



**Figure 6.4: Quantifying naphtha demand uncertainty**

The probability for the price to fall within  $\pm 3\sigma$  is expressed in terms of probability function  $p(y)$  as shown in Equation (6.3),

$$Pr\{-3\sigma \leq y \leq +3\sigma\} = \sum_{-3\sigma}^{+3\sigma} p(y) \leq 1.0 \quad (6.3)$$

Equation (6.3) also shows that in some exceptional scenarios, it is possible to have the price of naphtha falling outside the  $\pm 3\sigma$  range (i.e. extremely low prices or extremely high prices). The cumulative probability distribution  $\Phi$  further describes the probability of any variable  $Y$  to be equal or less than the value of  $y$ .  $\Phi$  is related to  $p(y)$  as follows:

$$\Phi = Pr\{Y \leq y\} = \sum_{Y \leq y} P(y) \quad (6.4)$$

A confidence level is usually assigned on the cumulative distribution function.

Quantifications for price and demand variations for gasoil are carried out similarly.

### 6.3.1 An Example for Quantifying Uncertainty

**Table 6.1. A 12-Period Historical Demand of Gasoil**

Period	1	2	3	4	5	6	7	8	9	10	11	12
Demand, $D$ (‘000 t)	43.8	42.8	41.9	44.1	45.8	44.8	43.4	44.5	42.2	42.5	41.8	42.2

Consider an arbitrary oil refinery. The refinery produces a range of fuel product, one of which is gasoil. A 12-period historical data for the demand of gasoil is shown in Table 6.1. The average demand over the whole horizon is calculated using Equation (6.1):

$$\bar{D} = \frac{\sum_{i=1}^n D_i}{n} = 43,300 \text{ t}$$

The standard deviation for the range of historical demand data is then calculated as per Equation (6.2):

$$\sigma = \sqrt{\frac{\sum_{i=1}^n (D_i - \bar{D})^2}{(n-1)}} = 1,290 \text{ t}$$

The frequency of demand occurrence within the range  $\pm 3\sigma$  is tabulated in Table 6.2.

**Table 6.2. Frequency of demand occurrence within  $\pm 3\sigma$**

Distribution	$-3\sigma$	$-2\sigma$	$-\sigma$	$+\sigma$	$+2\sigma$	$+3\sigma$
Frequency	0	0	2	8	2	0

The frequency of demand occurrence is also used to quantify probability of demand occurring within the range of  $\pm 3\sigma$ .

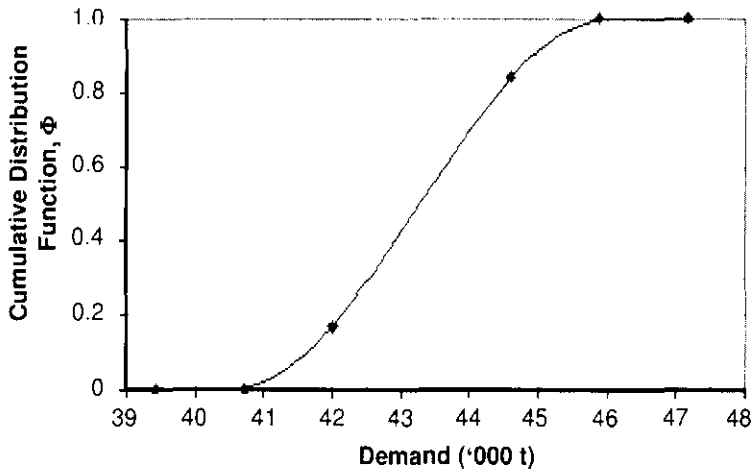


The probability function for each range of demand variation is calculated as per Equation 6.3. The result is shown in Table 6.3.

**Table 6.3. Probability function for the demand of a refinery product**

<i>Distribution</i>	$-3\sigma$	$-2\sigma$	$-\sigma$	$+\sigma$	$+2\sigma$	$+3\sigma$
$p(D)$	0	0	0.17	0.67	0.17	0

Equation (6.4) is further used to calculate the cumulative distribution function  $\Phi$ . Figure 6.5 shows the plot of  $\Phi$  as the demand varies. This plot gives the expected demand corresponding to any given percentile of  $\Phi$ .



**Figure 6.5: Cumulative distribution function for Example 6.3.1**

## **6.4 Solution Approaches to Problems with Uncertainty**

Problems in which some variables in the objective function or constraints are uncertain are typically addressed by stochastic programming approaches. The extent of uncertainty in the variables is often described by possible scenarios or by probability distribution. Although there are several available methods that can be used to describe the uncertainty, all of them allow for violation of constraints to occur (Ierapetritou and Pistikopoulos, 1996; Li, P. et. al., 2004; Li, W. et. al., 2004). Two common stochastic programming methods are the recourse model and the chance-constrained programming.

In the recourse model method, the violation of constraints is followed by a corrective action or recourse. For example consider a multi-period production plan where the production in some periods lags the demand. As a result, the demand constraint is violated and the production plan becomes infeasible. However, in the recourse model method, any amount of unmet demand during any period of the production is allowed by delivering it during the next possible period. This delivery situation is called backorder. Backorder, however, incurs a penalty charge which acts as a corrective measure in the recourse model method. The number of backorder occurrence can be described by possible scenarios.

The objective of production planning then is to find optimal operating strategy (i.e. raw materials selection, products allocation, process operating conditions, etc) that minimises the total production cost. Alonso-Ayuso, et. al. (2005) presented a two stage recourse-

model for the optimal product selection of a production planning problem under uncertainty. A two-stage recourse model can be generally formulated as follows:

$$\min \text{cost} = f(\mathbf{y}) + \sum_{\mathbf{s}} \left( Pr_{\mathbf{s}} \times \zeta \times \mathbf{y}_{\mathbf{s}} \right) \quad (6.5)$$

where  $f(\mathbf{y})$  is the deterministic cost function,  $\mathbf{s}$  is the number of scenarios,  $Pr$  is the probability of variable  $\mathbf{y}_{\mathbf{s}}$  occurring in scenario  $\mathbf{s}$ , and  $\zeta$  is the penalty charge for constraint violation during each scenario.

In the method of chance-constrained programming, uncertainty is modelled as a probability distribution as per Equation (6.3). The problem is then formulated as follows:

$$\begin{aligned} \min \text{cost} &= f(\mathbf{y}) \\ \text{s.t.} & \\ & Pr \left\{ \sum_I \mathbf{y}_I \leq \mathbf{y} \right\} \geq \beta_I \end{aligned} \quad (6.6)$$

where  $\mathbf{y}$  is the uncertain variable and  $\beta$  is the confidence level. Here, uncertainty in  $\mathbf{y}$  is treated as an additional constraint to the problem. Furthermore, let  $\Phi$  be the cumulative probability distribution of  $\mathbf{y}$  as per Equation (6.4). Then the constraint in Equation (6.6) is reformulated to

$$\sum_I \mathbf{y}_I \leq \Phi_I^{-1}(1 - \beta_I) \quad (6.7)$$

The right hand side of equation (6.7) is known for a given  $\beta_I$ . Then Equation (6.6) becomes a deterministic problem at some level of confidence  $\beta_I$ . The reformulation also enables the stochastic problem to be solved using existing deterministic optimisation method. The problem constraints can also be satisfied as a whole by assigning the same

confidence level  $\beta_j = \beta$  for all  $y_j$ . The following example shows how the chance-constraint programming method is used to solve a simple production planning problem.

### 6.4.1 An Example of Production Planning under Uncertainty

Consider an arbitrary petrochemical plant producing  $y$  t of product from a single raw material to meet demand  $D$ . Assume the raw material cost is  $0.6 \times y$  and the operation cost is  $0.2 \times y$ . The plant must decide the amount of product to make in order to meet the demand at minimum total cost. Furthermore, the demand  $D$  is uncertain. From historical demand data, it is expected that the demand follows a normal distribution curve with average  $\bar{D} = 43.3$  t and standard deviation  $\sigma = 1.3$ .

The production planning problem is then formulated as follows,

$$\begin{aligned} \min \text{ cost} &= 0.6y + 0.2y \\ \text{s.t.} & \\ &Pr\{y \geq \tilde{D}\} \geq \beta \\ &y \geq 0 \end{aligned}$$

where  $\tilde{D}$  is the uncertain demand. Let the cumulative distribution function for the uncertain demand,  $\Phi$ , be

$$\Phi = \begin{cases} 0 & \text{for } D < -\sigma \\ 0.17 & \text{for } -\sigma \leq D < +\sigma \\ 0.84 & \text{for } +\sigma \leq D < +2\sigma \\ 1.0 & \text{for } D \geq +2\sigma \end{cases}$$

Hence, the stochastic problem is reformulated into its deterministic equivalence,

$$\begin{aligned}
 \text{min cost} &= 0.6y + 0.2y \\
 \text{s.t.} & \\
 &y \geq \Phi^{-1}(\beta) \\
 &y \geq 0
 \end{aligned}$$

where  $\Phi^{-1}(\beta)$  is the inverse cumulative distribution function of the uncertain demand.

Selecting  $\beta = 0.95$ , then  $\Phi^{-1}(\beta) = 45.4$ . Solving the linear problem gives  $y = 45.4$  and  $\text{min cost} = \$36.35$ .

### **6.5 Feasibility Analysis of Integrated Production Planning under Uncertainty**

Flexible production planning in an oil refinery and a petrochemical plant can be achieved if the plant is able to operate feasibly over a range of uncertain product demand and prices. Given an optimum integrated production plan generated with demand and prices certainty, the feasibility analysis is carried out by allowing the demand and price parameters to vary according to their probability distribution functions. Probability distribution function is generated from historical data as discussed in Section 6.3. Furthermore, the cumulative distribution functions for the uncertain parameters are also determined. Incorporating the uncertainty as constraints in the problem formulation yields a probabilistic integrated production planning problem. To reformulate the problem into its deterministic equivalent, a confidence level is assigned to the probabilistic constraint. The resulting problem is then solved using approaches discussed in Section 6.4.

The results are then checked for constraints violations. If no violations occur, then the integrated production plan is said to be flexible. Otherwise, the constraint violations are determined and corrective actions are carried out. Generation of corrective actions can be performed systematically. For example let the constraint on inventory level as per Equation (5.13) shown in the previous chapter be represented by

$$g(y) \geq 0 \quad (6.8)$$

Due to uncertainty in demand, Equation (6.8) may be relaxed by incorporating a slack variable  $\Delta g$ . Hence the inequality constraint is transformed into the following equality constraint:

$$\begin{aligned} g(y) + \Delta g &\geq 0 \\ \Delta g &\geq 0 \end{aligned} \quad (6.9)$$

The optimisation will attempt to satisfy  $g(y)$ . However, if  $g(y)$  alone cannot satisfy Equation (6.9), then any shortfall will be assigned to the slack variable  $\Delta g$ . There is also a penalty cost  $r$  incurred for  $\Delta g$ . The penalty is incorporated into the objective function as follows:

$$\min \text{cost} + r \cdot \Delta g \quad (6.10)$$

Penalty cost  $r$  can be set to a very large arbitrary value such that the selection of  $\Delta g$  will be made just sufficient for a feasible solution to be reached. The additional penalty incurred is then equal to the cost of flexibility.

Figure 6.6 summarises the steps taken to analyse the feasibility of integrated production under uncertainty.

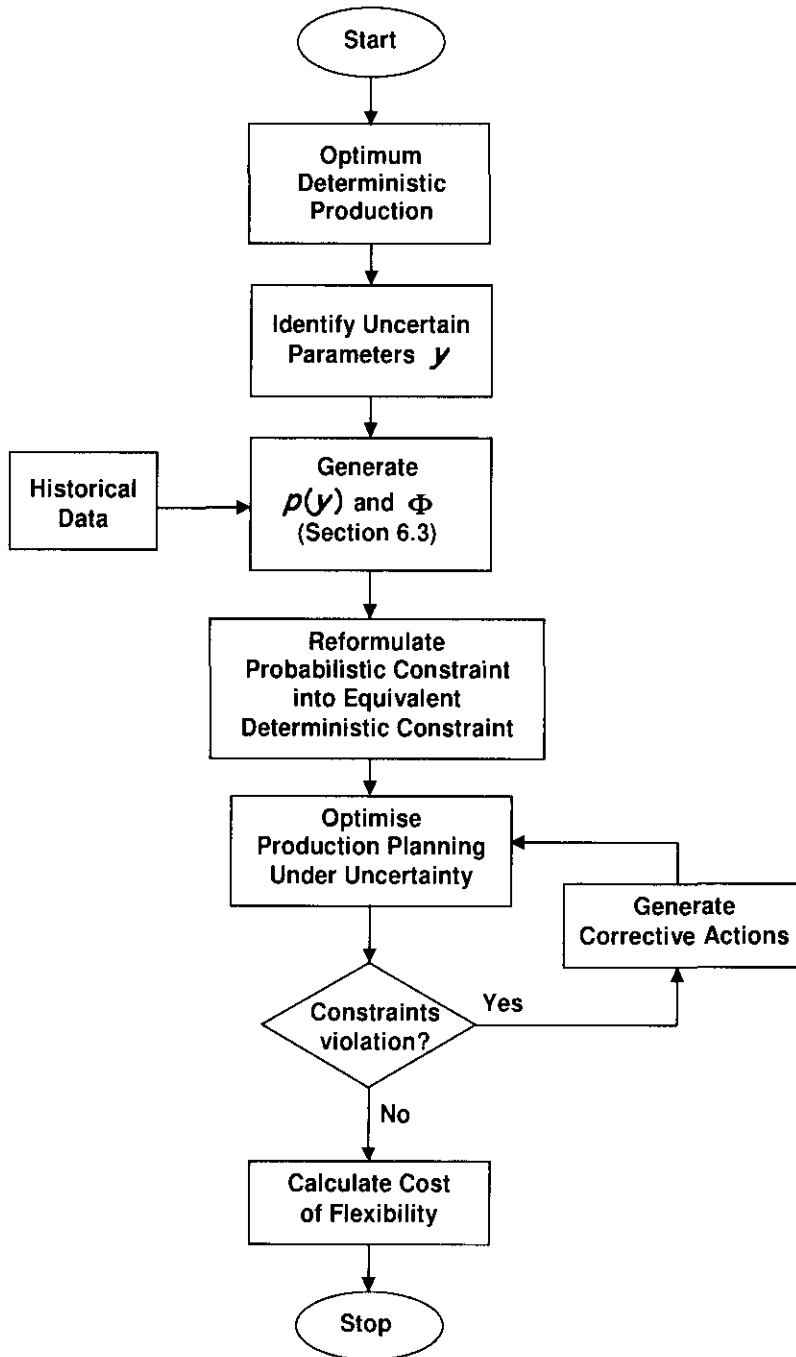


Figure 6.6: Approaches to the analysis of a flexible integrated production plan

### 6.6 Case Study 3: Flexible Integrated Production under Uncertain Demand and Prices

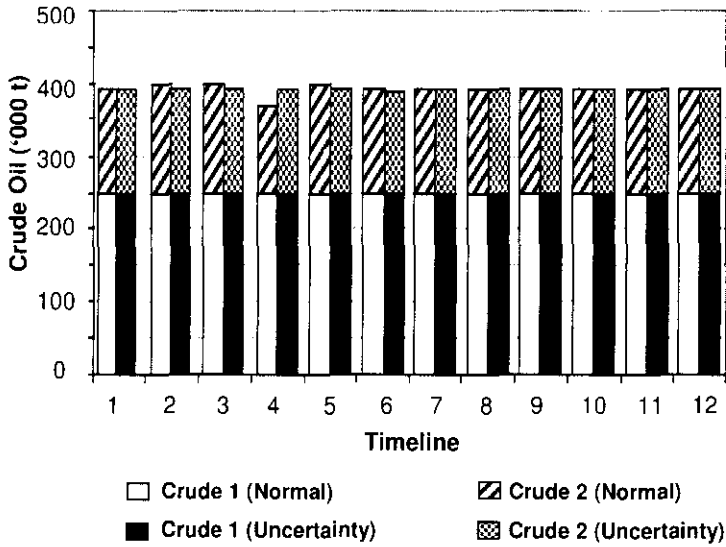
This case study is carried out to analyse the effect of uncertainty in demand and prices on the flexibility of planning for integrated production. To avoid problem complexity, only the variation of demand and prices of refinery naphtha is considered. Historical data for variations in naphtha demand and prices are shown in Figure 6.1. The probability distribution function and the cumulative distribution function for both naphtha demand and prices are tabulated in Table 6.4. All other constraints on feed quality, process capacity and product distributions remain the same as those presented in Table 4.2.

**Table 6.4. Data for uncertainty in naphtha demand and prices**

	Demand (D)	Price ( $\Pi$ )
<b>Average</b>	41.9 t/h	\$195.16/t
<b>Standard Deviation</b>	1.3 t/h	\$42.92 /t
<b>Probability Distribution</b>	$-\sigma = 0.33$ $+\sigma = 0.67$	$-2\sigma = 0.10$ $-\sigma = 0.53$ $+\sigma = 0.25$ $+2\sigma = 0.08$ $+3\sigma = 0.03$
<b>Cumulative Distribution</b>	$\Phi = \begin{cases} 0 & \text{for } D \leq -\sigma \\ 0.33 & \text{for } -\sigma \leq D < +\sigma \\ 1.00 & \text{for } D \geq +\sigma \end{cases}$	$\Phi = \begin{cases} 0 & \text{for } \Pi \leq -2\sigma \\ 0.10 & \text{for } -2\sigma \leq \Pi < -\sigma \\ 0.63 & \text{for } -\sigma \leq \Pi < +\sigma \\ 0.88 & \text{for } +\sigma \leq \Pi < +2\sigma \\ 0.96 & \text{for } +2\sigma \leq \Pi < +3\sigma \\ 1.00 & \text{for } \Pi \geq +3\sigma \end{cases}$

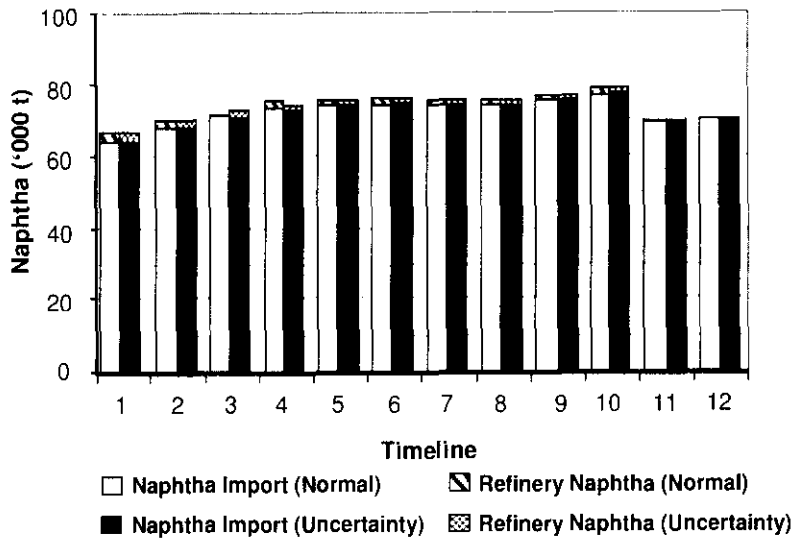


Optimum crude selection between normal production planning and planning under uncertainty in demand and prices is shown in Figure 6.7. For the production planning with uncertainty, there is a significant increase in crude 2 feed during period 4.

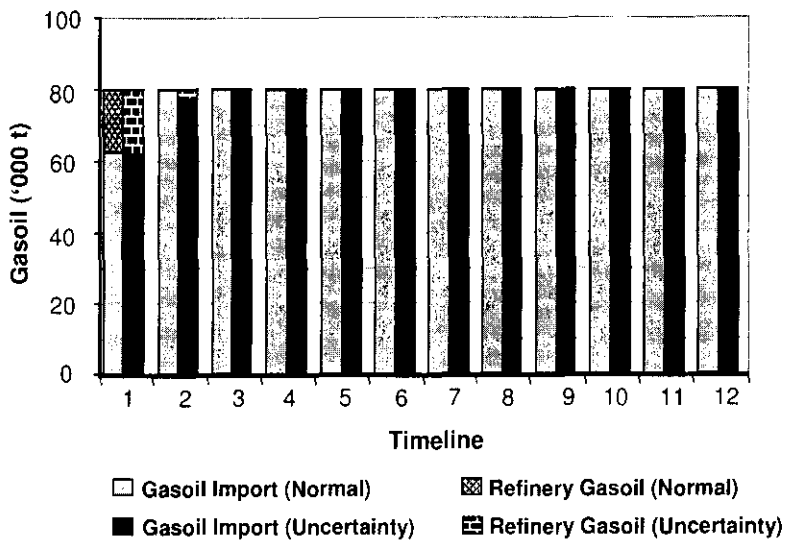


**Figure 6.7: Comparison of crude oil feed profiles between normal production planning and planning under uncertainty**

This behaviour can perhaps be explained as a solution strategy to adapt with the uncertain demand and prices. For the petrochemical plant, the same behaviour is noticeable during period 3 for naphtha feed. Gasoil feed mix shows additional refinery gasoil integration during period 2. The feed profiles for the petrochemical plant are shown in the Figures 6.8 and 6.9 respectively.

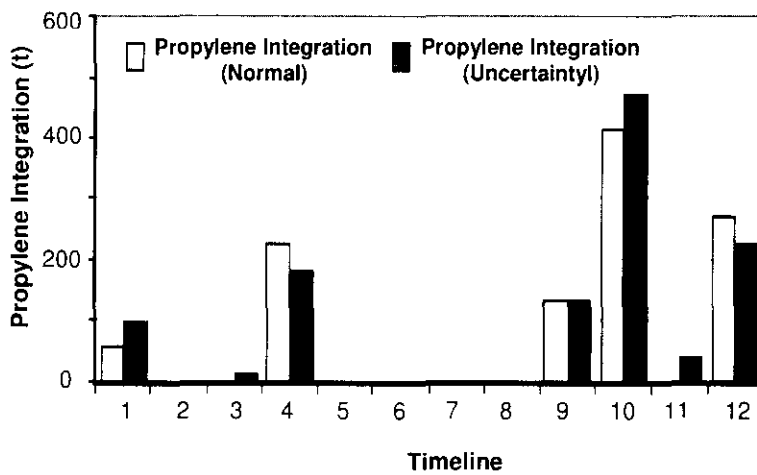


**Figure 6.8: Comparison of naphtha feed profile between normal production and planning under uncertainty.**



**Figure 6.9: Comparison of gasoil feed profile between normal production and planning under uncertainty.**

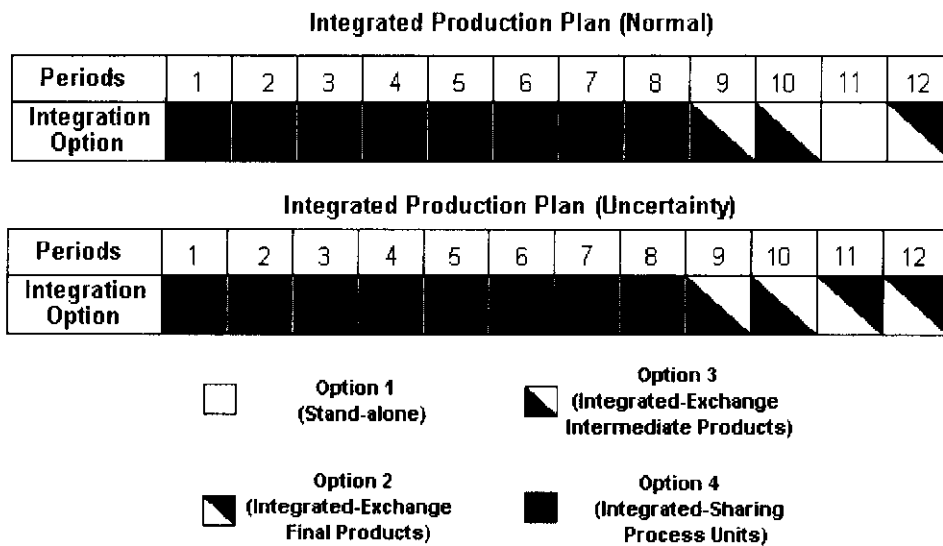
Annual naphtha integration during production planning under uncertainty is 9,665 tons. This figure is nearly a 5% drop from the quantity of naphtha integrated during normal integrated production planning. However, gasoil integration during production planning under uncertainty increases from 17,641 tons during normal production planning to 20,914 tons during planning under uncertainty. Annual propylene integration increases by more than 21% during planning under uncertainty. The amount of propylene integration during normal integrated production planning is 973 tons. During integrated production planning under uncertainty, the amount of propylene integration is 1182 tons. The integration profile for integration of propylene products is shown in Figure 6.10.



**Figure 6.10: Propylene integration during normal production planning and planning under uncertainty.**

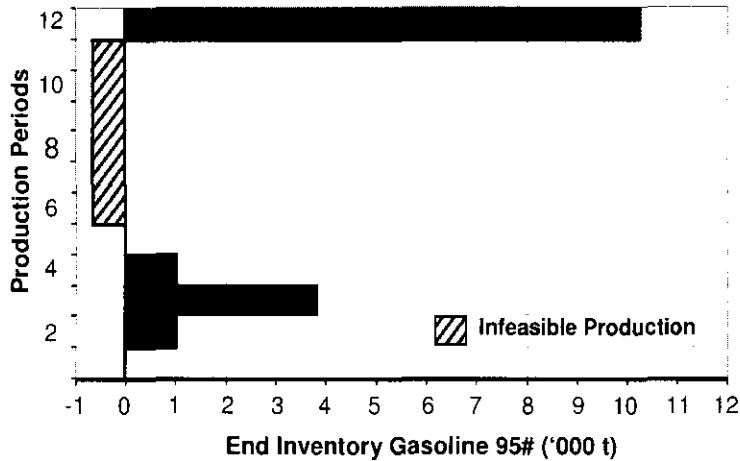
The integration of aromatic extraction unit shows little change on the amount of pygas sent to refinery (about 0.8%). This behaviour can perhaps be explained by the fact that pygas is not a major commodity product. Consequently, pygas product is not typically affected by the fluctuation in demand and prices.

The overall integration profiles during normal production planning and during planning under uncertainty are compared in Figure 6.11. The profiles show an increase in the number of integrated production strategy employed during planning under uncertainty. The optimum result perhaps points to the benefits of integration towards reducing the impact of uncertainty.



**Figure 6.11: Comparison of integrated production during normal planning and during planning under uncertainty.**

Figure 6.12 further illustrates the inventory profile for gasoline 95# during planning under uncertainty. The region shaded with upward diagonal lines shows infeasible production. Due to uncertainty in demand, there is an expected shortage of about 600 tons of gasoline 95# product from the oil refinery during period 6. Fortunately, detection of possible infeasibility through this analysis allows corrective actions to be taken early in the planning stage.



**Figure 6.12: Infeasible production of gasoline 95# during planning under uncertainty.**

There are two possible options to maintain flexibility in the production plan and continue the feasible operations under uncertainty. The first option is to relax the demand constraint. For the case of gasoline 95# production, the relaxation of constraints can be implemented if back-order is allowed. Since large gasoline 95# inventory is expected during period 12, the shortage in period 6 can be delivered in period 12. Figure 6.13 illustrates a feasible integrated production strategy under uncertainty with a relaxed constraint. However, the oil refinery would typically be expected to pay a fixed penalty per ton of shortage per period.

When back-order is not allowed, then the second option is to increase the initial inventory during the start of the first production planning period. As shown in Figure 6.14, the initial inventory during the start of period 1 is increased to ensure continued feasibility of integrated production strategy under uncertainty. However, there are also a couple of

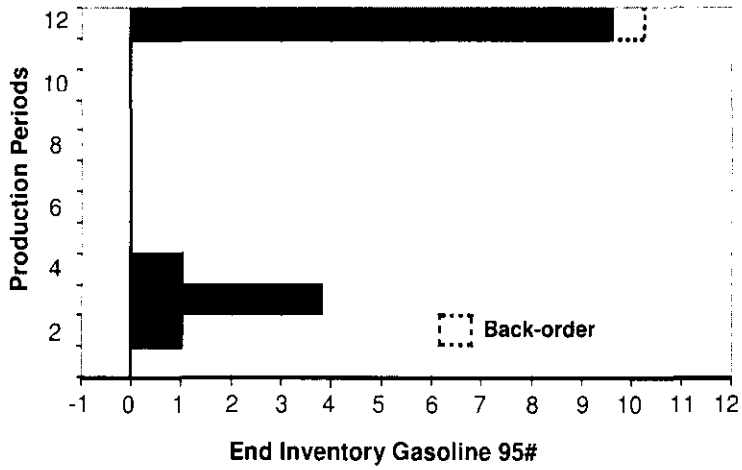


Figure 6.13: Feasible production of gasoline 95# during planning under uncertainty with relaxed demand constraint.

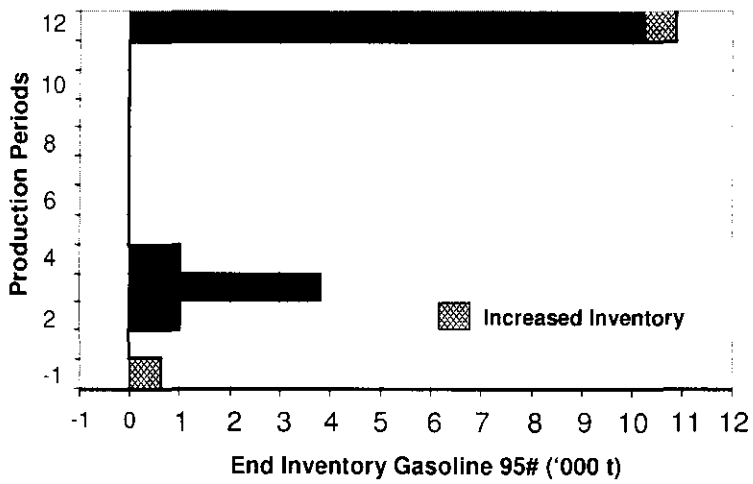


Figure 6.14: Feasible production of gasoline 95# during planning under uncertainty with increased starting inventory during period 1.

additional inventory costs involved. The first cost is incurred during the end period -1 and the second cost occurs at the end of period 12. The choice of which options to select depends on the constraints of back-order and the overall cost incurred between the two options.

The computational information for optimising integrated production with uncertainty is tabulated in Table 6.5. The problem of optimisation with uncertainty uses a little over 12% more iterations than the normal problem (i.e. problem with certain demand and prices). However, the resource usage for the problem with uncertainty is within the same magnitude as that of the normal problem. Consequently, the problem with uncertainty has been solved within an acceptable computational performance.

**Table 6.5: Comparison of performance between normal production planning and planning under uncertainty**

	<b>Optimisation (Uncertainty)</b>	<b>Optimisation (Normal)</b>
<b>Number of Variables</b>	3,368	3,368
<b>Iteration Count</b>	25,971	23,138
<b>Resource Usage (s)</b>	81	77

## **6.7 Summary**

In this chapter, the issue of flexibility of integrated production planning is discussed. Flexibility is achieved when the planned integrated production continues to be feasible under uncertainty in parameters like demand and prices. The probability distribution for demand and prices can be approximated from historical data. Uncertainty can be incorporated into integrated production planning as an additional optimisation constraint. A case study is presented to compare integrated production under normal planning and planning under uncertainty. The overall integration profile shows increased integration during planning under uncertainty. This result shows that integration increases the flexibility of plant production under uncertainty. Furthermore, through this analysis, any possible infeasibility can be detected and corrective actions can be carried out as soon as possible. The additional cost incurred in carrying-out the corrective actions is the cost of maintaining flexibility for the integrated production strategy.



## **6.8 References**

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## ***Chapter 7 Conclusions and Future Work***

7.1 Conclusions and Significance.....	148
7.2 Future Work.....	151

## ***7.1 Conclusions and Significance***

This work explores integrated production as a strategy for oil refineries and petrochemical plants to remain competitive in a globalised economy. The potential for integrated production strategy to increase the profitability and to enhance the production flexibility of an integrated oil refinery and petrochemical plants is analysed. Strategies for an efficient implementation of the integrated production are also developed.

Oil refining and petrochemical industries realise the significant potential of an integrated production strategy on their profitability. Since the turn of the new millennium, many large oil refining and petrochemical plants are making integration as a key feature in many of their new projects. The industries themselves are taking the lead by carrying out the studies on integrated productions. However much of the reported work are based on linear models for a single product integration within the same company itself. It is perhaps the size and the complexity of the problem coupled with the attitude of secrecy in the industries that discourage the academic research in this area. This work therefore attempts to address the issue from outside the industry circle.

A general modelling approach comprising an overall production planning at the site level and an individual yield correlation at the process level is developed. Yield correlations are simple, mostly non-linear, models that are able to predict the production profiles of both oil refinery and petrochemical plant processes with sufficient accuracy. This strategy results in the overall production planning optimisation problem to be easily modelled and

managed. The overall problem is formulated as a non-linear programming (NLP) problem.

Production planning problems are optimised for maximum profit margin while meeting the constraints on product demands, process unit capacities, and the limitations on the process unit operating conditions. Integrated production adds the opportunity to increase the individual plant's profit by exploiting the flows of material between the plants. Shifting of propylene, naphtha, gasoil and pygas to the integrated plant is shown to significantly reduce the final and intermediate product inventories. In addition, it also provides added revenue to the selling plant and reduces the materials cost for the purchasing plant. The pricing mechanism used in determining the price of exchanging materials is based on the cost-plus approach to determine the plant posted price. The price of exchanging materials can then be decided with reference to the plant posted price. The agreed price is the one that would give the selling plant a reasonable profit and the purchasing plant a reasonable discount on the exchanged materials. As a result, the integrated plants benefit from lower costs and higher profits than in the stand-alone production strategy.

A number of implementation issues are also addressed in this work. These include determining the necessity to integrate production before performing detail implementation tasks. Detail implementation tasks include generating options of integrated production network and finding the optimum production plan for each option. Sequential optimisation approach is proposed to reduce the computational complexity in

handling large NLP problems. The modularity of the solution approach also enables a third party interaction model to be easily incorporated. The role of the interaction model is to bridge the information required for generating an optimum integrated production plan while protecting proprietary process models of the individual plant. The computational performance of the sequential optimisation approach is also found to be better than the computational performance of the simultaneous optimisation approach.

The flexibility of integrated production planning is analysed for its ability to be feasible under a range of uncertain parameters like demand and prices. Using historical data to provide the probability distribution, uncertainty in demand and prices are incorporated into integrated production planning as additional optimisation constraints. Integrated production is shown to increase the flexibility of production planning under uncertainty. Infeasible production can also be detected at an early stage which allows for corrective actions to be carried out before the start of the actual production planning period. The cost of maintaining flexibility for the integrated production strategy is calculated from the additional cost incurred in carrying-out the corrective actions.

The significance of this work is that it provides a better understanding on the opportunities and issues involved in implementing an integrated production strategy. Integrated production provides more degrees of freedom for plants to increase their profitability and flexibility. The understanding gained from this study is valuable because it is not possible to empirically test-run the integration in real companies. Case studies

show the effectiveness of the strategy and its potential to enhance the competitiveness of an integrated oil refineries and petrochemical plants in a globalised economy.

## **7.2 Future Works**

This research work has found that integration of production between plants offer much potential for the enterprise to gain mutual benefits in terms of profitability and flexibility. However, much work is still required to fully understand the full extent of the benefits that can be harnessed from an integrated production strategy.

Firstly, to complete the real industrial application of integrated production planning, the issues of forecasting and scheduling need to be addressed. On one end, forecasting requires taking a more detail approach to determining the demand and price uncertainty. Key variables affecting demand and prices, for example seasonal change, number of active plants, number of oil wells, etc., need to be incorporated in the forecasting model. On another end, scheduling requires more detail timing aspects to modelling. The level of inventory needs to be correlated to the timing of ship berth, product delivery, marketing and sales level, etc.

Next, hydrogen is an issue that requires special attention in the integrated production strategy. Both the steam reforming and steam cracking processes produce considerable

quantity of hydrogen as by-products. As demand for hydrogen increases in refinery processes to meet stricter environmental regulations, it would be interesting to extend the hydrogen network beyond the OSBL of the oil refineries and into the petrochemical plants.

Finally, total integration between complimentary plants may also be considered in the future. For example, oil refineries and petrochemical plants may want to exploit the simultaneous energy and materials integration between them. This inadvertently results in a very large problem of multiple complexities. However, the advancement of computational power nowadays may provide some aids in tackling this complex problem.

***Appendix A***

***Cost Data***



1. Cost of crude oils (\$/t)  
Crude 1 = 125  
Crude 2 = 120
2. Cost of steam cracker feeds (\$/t)  
Naphtha = 185  
Gasoil = 160
3. Price of oil refinery products (\$/t)  
LPG = 185  
Propylene = 400  
Naphtha = 180  
Jetfuel = 190  
Gasoline 93# = 190  
Gasoline 95# = 195  
Diesel = 180  
Benzene = 300  
Toluene = 300  
Xylene = 300
4. Price of petrochemical plant products (\$/t)  
Ethylene = 450  
Propylene = 400  
Butadiene = 300  
C4mix = 180  
Pygas = 150
5. Price of integrated products (\$/t)  
Propylene = 152  
Naphtha = 167  
Gasoil = 154  
Pygas = 127

6. Typical utility consumption for major unit operations

	Crude Distillation Unit	Catalytic Reformer Unit	Fluid Catalytic Cracker Unit	Naphtha Steam Cracker Unit
Fuel	-	2360 MJ/t	2422 MJ/t	4866 MJ/t
Steam	-	123 kg/t	234 kg/t	428 kg/t
Power	1.67 kWh/bbl	16.4 kWh/t	11.7 kWh/t	26.8 kWh/t
Water	0.43 m3/bbl	11.1 m3/t	10.5 m3/t	13.39 m3/t

7. Utility costs

Fuel = \$1.90/GJ  
 Steam = \$3.25/t  
 Power = \$5.00/hundred kWh  
 Water = \$5.00/thousand m3

## ***Appendix B***

### ***Yield Correlations for Refinery and Petrochemical Process Units***

## B1. Crude Distillation Unit

Let,  
 AP : Aniline point (°C)  
 API : API gravity  
 CF : Characterisation factor  
 FCD : Products flowrate crude distillation (t/h)  
 FCrude : Crude feed flowrate (t/h)  
 i : Set of refinery product types  
 j : Set of product specifications  
 n : Set of production periods  
 RON : Research octane number  
 SG : Specific gravity  
 VABP : Volumetric average boiling point (°C)

Then,

Production from Crude Distillation (t/h)

$$FCD(i,n) = CrudeTBP('Yield',i)*FCrude(n)$$

CrudeTBP(j,i)

Cut	Lt.Gas	Lt.Naphta	Naphtha	Kerosene	Diesel	Gasoil	Residue
Yield	0.0309	0.0518	0.2143	0.1059	0.1593	0.2358	0.2021
SG	0.3000	0.7167	0.7600	0.7900	0.8200	0.8600	0.9200
API			54.7		41.1	33.0	
RON		63	55				
Cetane					56		
CF				11.83	11.83	11.83	12.00
AP				21.70		65.56	48.89
VABP						417.2	700.0
Naphtene			0.4500				
Aromatics			0.0500				
Sulfur		8.65e-5	1.08e-4	4.02e-4	5.44e-4	5.84e-4	1.00e-2
Nitrogen					2.18e-5	3.80e-4	4.00e-3

## B2. Aromatics Production Unit

Let,

delta : Reformate split between fuel and aromatic products  
FRef : Products from refinery (t/h)  
i : Set of refinery product types  
n : Set of refinery production periods  
N2A : Content of naphthene plus two aromatics in CRU feed (wt%)  
PChPygas : Flowrate pygas from petrochemical (t/h)  
RONCRU : Severity of catalytic reformer operations  
xCR : Raw yields catalytic reformer

Then,

Benzene Production (t/h)

$$FRef('Benzene',n) = \text{delta}(n) * xCR('A6',n) * xCR('Reformate',n) * FeedCRU(n)$$

Toluene Production (t/h)

$$FRef('Toluene',n) = \text{delta}(n) * xCR('A7',n) * xCR('Reformate',n) * FeedCRU(n)$$

Xylene Production (t/h)

$$FRef('Xylene',n) = \text{delta}(n) * xCR('A8',n) * xCR('Reformate',n) * FeedCRU(n)$$

C6 Aromatics Yield (wt%)

$$xCR('A6',n) = (0.00007195 * N2A(n) / (-0.0003553 + 0.0003712 * \text{EXP}(-0.0001816 * \text{RONCRU}(n))) + 0.6903) / 100$$

C7 Aromatics Yield (wt%)

$$xCR('A7',n) = (-0.01695 * \text{RONCRU}(n)**2 - 34.3912 * N2A**2 + 3.5769 * \text{RONCRU}(n) - 166.1344) / 100$$

C8 Aromatics Yield (wt%)

$$xCR('A8',n) = (-0.02863 * \text{RONCRU}(n)**2 - 52.2832 * N2A**2 + 5.7230 * \text{RONCRU}(n) - 252.5582) / 100$$

C9+ Aromatics Yield (wt%)

$$xCR('A9plus',n) = (-0.03318 * \text{RONCRU}(n)**2 - 52.3693 * N2A**2 + 6.1306 * \text{RONCRU}(n) - 252.9738) / 100$$

Non-Aromatics Yield (wt%)

$$xCR('NonAro',n) = (1 - xCR('A6',n) - xCR('A7',n) - xCR('A8',n) - xCR('A9plus',n))$$

Reformate Production (t/h)

$$F_{\text{Ref}}(\text{Reformate},n) = (1-\text{delta}(n)) * (\text{xCR}(\text{Reformate},n) / \text{SUM}(\text{xCR}(i,n) * \text{Feed1CRU}(n)) + \text{delta}(n) * ((\text{xCR}(\text{A9plus},n) + \text{xCRNonAro}(n)) * \text{xCR}(\text{Reformate},n) / \text{SUM}(\text{xCR}(i,n) * \text{FeedCRU}(n)))$$

C7 Pygas Production (t/h)

$$\text{PygasC7}(n) = 0.23 * \text{PChPygas}(n);$$

C8 Pygas Production (t/h)

$$\text{PygasC8}(n) = 0.13 * \text{PChPygas}(n);$$

C9+ Production (t/h)

$$\text{PygasC9plus}(n) = 0.41 * \text{PChPygas}(n)$$

Non-Aromatics Pygas Production (t/h)

$$\text{PygasNonAro}(n) = 0.22 * \text{PChPygas}(n);$$

### **A3. Steam Cracker Production Unit**

Let,

IM : Feed Molecular Index  
IS : Steam Cracker Severity Index  
m : Set of petrochemical plant production periods  
k : Set of petrochemical product types  
xSC : Raw yield from steam cracker (wt%)  
FNaphtha : Naphtha feed flowrate (t/h)

Then,

Fuel Gas Yield (wt%)

$$xSC('FuelGas',m) = 1/(1.5868902*IM + 51.6080333*exp(-IS(m)))$$

Ethylene Yield (wt%)

$$xSC('Ethylene',m) = 1/(13.5157187*IM + 10.28963808*exp(-IS(m)) - 39.0900618)$$

Propylene Yield (wt%)

$$xSC('Propylene',m) = 0.014539*IM + IS(m)*(0.027805 - 0.004819*IS(m)) + 0.076915$$

Pygas Yield (wt%)

$$xSC('Pygas',m) = 0.07321*IM + IS(m)*(0.2919 - 0.05121*IS(m)) - 0.389435$$

Fuel Gas Production (t/h)

$$FPCh('FuelGas',m) = xSC('FuelGas',m)/SUM(xSC('k',m)*FNaphtha(m))$$

Ethylene Production (t/h)

$$FPCh('Ethylene',m) = xSC('Ethylene',m)/SUM(xSC('k',m)*FNaphtha(m))$$

Propylene Production (t/h)

$$FPCh('Propylene',m) = xSC('Propylene',m)/SUM(xSC('k',m)*FNaphtha(m))$$

Pygas Production (t/h)

$$FPCh('Pygas',m) = xSC('Pygas',m)/SUM(xSC('k',m)*FNaphtha(m))$$