Cranfield University

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PLANNING FOR THE INTEGRATED REFINERY SUBSYSTEMS

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Co-Supervisor: Prof. Hoi Yeung

June 2012

This thesis is submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy

Abstract

In global energy and industrial market, petroleum refining industry accounts for a major share. Through proper planning and the use of adequate mathematical models for the different processing units, many profit improving opportunities can be realized. The increasing crude oil price has also made refining of crude oil blends to be a common practice. This thesis aims to provide useful insight for planning of the integrated refinery subsystems. The main subsystems referred to are (1) The crude oil unloading subsystem (2) The production and product blending subsystem and (3) The product distribution subsystem.

Aspen HYSYS® was first used to develop a rigorous model for crude distillation unit (CDU) and vacuum distillation unit (VDU). The rigorous model was validated with pilot plant data from literature. The information obtained from the rigorous model is further used to develop a model for planning of the CDU and VDU. This was combined with models (obtained from empirical correlations) for fluid catalytic cracker (FCC) and hydrotreater (HDT) units to form a mathematical programming planning model used for refinery production and product blending subsystem planning. Since two different types of crude were considered, the optimum volumetric mixing ratio, the sulphur content at that mixing ratio and the CDU flow rate were determined.

The yields fraction obtained from the rigorous model were then used to generate regression model using least square method. The sulphur composition of the crude oil was used as independent variable in the regression model. The generated regression models were then used to replace the regular fixed yield approach in a refinery planning model and the results compared. From the results obtained, the proposed method provided an alternative and convenient means for estimating yields from CDU and VDU than the regular fixed yield approach.

The proposed aggregate model for the production and products blending subsystem was integrated with the modified scheduling model for the crude unloading subsystem developed by Lee et al. (1996) and products distribution model developed by Alabi and Castro (2009) for refinery planning. It was found that the regression model could be integrated in a refinery planning model and that the CDU flow rate was maximised as compared to the non- integrated system.

Keywords: Refinery planning, linear programming, optimization, linear regression, process modelling

Acknowledgements

I hereby extend my innermost gratitude to Dr. Meihong Wang my supervisor. Meihong, this thesis benefited immensely from your guidance, tolerance, your excellent grasp of what was important and your attention to detail. You were always available when I needed help and your support and encouragement kept me going throughout the difficult times. I would also like to extend my appreciation to my co-supervisor, Professor Hoi Yeung for his high level critics and ingenuity all through the cause of this work. Hoi, you are not just a supervisor, but a friend and a confidant. I really appreciate you.

My sincere appreciation goes to Dr Lazaros Papageorgiou and Dr Songsong Liu at Department of Chemical Engineering, University College London (UCL) for their candid contribution in making this work a huge success.

I would like to extend my appreciation to Dr 'Keluo Chukwuogo, the Managing and Technical Director of Boskel Nigeria Ltd. for all his support and encouragements. 'Keluo, if not for your prod towards self-development, PhD would not have been considered. I thank you for the motivation.

My personal gratitude is extended to my colleagues, Chet, Mubarak, Alhaji Aminu, Aminu Hamisu, Habeeb, Yemi, and most importantly Adekola for your continuous support and encouragement all through the period of this work.

The VC Bedford family, you will never be forgotten, especially my Mummy in the Lord Pastor Christina Emmanuel-Odiachi for your sincere and continuous encouragements and prayers all through the tough times. May the Lord continue to pour his fresh oil upon you and your family will always remain in the hollow of his palm.

Enough thank you cannot be said to my siblings and my mum for their endless prayers. Special thank you to my sister fondly called Nulia and her family for all effort made to see that this work was a success.

My heartfelt appreciation to my darling and loving husband (Obim) for all the sacrifices you offered for this journey to come true. You denied yourself of a lot of things for this work to move on. Your encouragement was second to none; I am saying thank you to the best Daddy in the world. Also to my beautiful daughters Chidera Adaeze Nkeiruka Ejikeme and Fechi Kosisochukwu Chisom Ejikeme for all their support and understanding all through the hard times. Your birthday celebrations were denied so that mummy can meet up with her work. From my heart, I say thank you and I love you all so much.

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Abbreviations

AGO Atmospheric Gas Oil

CDU Crude Distillation Unit

VDU Vacuum Distillation Unit

FCC Fluid Catalytic Cracking

HDT Hydrotreater

VE Vessels

CT Charging Tank

API American Petroleum Institute

TBP True Boiling Point

$ASTM$ American Society for Testing and Materials

bbl Barrels

$MILP$ Mixed integer linear programming

$MINLP$ Mixed integer non-linear programming

NLP Non-linear programming

LP Linear programming

EBP End Boiling Point

IBP Initial Boiling Point

EIA Energy Information Administration

FG Fuel Gas

FO Fuel-Oil

GO Gross Overhead

HN Heavy Naphtha

HD Heavy Distillate

LN Light Naphtha

LD Light Distillate

BR Bottom Residue

$GAMS$ General Algebraic Modelling Systems

GB Gasoline Blend

$Gasb$ Gasoline product

$HVGO$ High Vacuum Gas Oil

$LVGO$ Low Vacuum Gas Oil

LPG Liquefied Petroleum Gas

NBP Normal Boiling Point

$PIMS$ Process Industry Modelling Systems

$RPMS$ Refinery and Petrochemical Modelling Systems

Nomenclature

Set/indices

VE = {v =1, 2…V/ crude oil vessel}

ST = {i =1, 2…I/ storage tanks}

CT = {j =1, 2…J/charging tanks}

COMP = {k =1,2…K/ crude oil components}

CDU = {l = 1,2…L/crude distillation units}

Time = {t =1,2…T/ Time Horizon}

Time = {m =1,2…m/ Time Horizon}

$VS_{i,t}$:	Volume of crude oil in storage tank i at time t
$VSmax_i$:	Storage tank i maximum capacity.
$VB_{j,t}$	Volume of crude oil in charging tank j at time t
$VSmin_i$:	Storage tank minimum capacity.
$VBmax_j$:	Charging tank maximum capacity.
$VBmin_j$:	Charging tank minimum capacity
$CUNLD_v$:	Unloading cost for vessel v
$CSETUP_j$:	Charging tank changeover cost
$CINVST_i$	Inventory cost for storage tanks i per unit time per unit volume
$CINVCT_j$	Inventory cost for charging tanks j per unit time per unit volume
$KBmin_{j,k}$:	Minimum concentration of component k in the blended crude oil of charging tank j.
$KBmax_{j,k}$:	Maximum concentration of component k in the blended crude oil of charging tank j.
$KSmin_{i,k}$:	Minimum concentration of component k in storage tank i.
$KSmax_{i,k}$:	Maximum concentration of component k in storage tank i.

DM_j:	Demand of blended or mixed crude oil j by CDU within the scheduling horizon
$FVS_{v,i,t}$	Volumetric flow rate from vessel v to storage tank i at time t.
$FVSmax_{v,i,t}$	Maximum crude oil rate from vessel v to one storage tank i.
$FVSmin_{v,i,t}$:	Minimum crude oil rate from vessel v to one storage tank i. In this situation its assumed 0
$FSB_{i,j,t}$	Volumetric crude oil rate from storage tank i to one charging tank j.
$FSBmax_{i,j,t}$	Maximum crude oil rate from storage tank i to one charging tank j.
$FSBmin_{i,j,t}$	Minimum crude oil rate from storage tank i to one charging tank j
$FBC_{j,l,t}$	Volumetric flow rate from charging tank j to CDU l at time t
$FBCmax_{j,l,t}$	Maximum crude oil rate from charging tank j to CDU l
$FBCmin_{j,l,t}$	Minimum crude oil rate from charging tank j to CDU l
$VV_{v,t}$	Volume of crude oil in vessel v at time t
$KY_{v,i,t}$	Binary variable to denote if storage tank i is receiving crude from vessel v.
$KYS_{i,j,t}$	Binary variable to denote if charging tank j is receiving crude from storage tank i
$KYB_{j,l,t}$	Binary variable to denote if CDU l is receiving mixed or blended crude j,g from charging tank j
$KFVS_{v,i,k,t}$	Volumetric flow rate of component k from vessel v to storage tank i at time t.
$KFSB_{i,j,k,t}$	Volumetric flow rate of component k from storage tank i to one charging tank j.
$KFBC_{j,l,k,t}$	Volumetric flow rate of component k from charging tank j to CDU l at time t
$VBK_{j,k,t}$	Volume of component k in charging tank j at time t

TF_v	Time for vessel v to begin unloading
TL_v	Time for vessel v to finish unloading
$TARR_v$	Vessel v arrival time
TDP_v	Vessel v departure time
$XR_{i,t}$	Binary variable to denote storage tank I holding at time t
PMD	Penalty for holding tank i
$COST$	Total optimal operational cost
α_j	Parameter for demand violation for mixed crude j
β_l	Parameter defined by the user that determines the interval to interval variation for CDU l throughput.
$Z_{j,g,l,t}$	Binary variable to denote that CDU l switches from charging tank j to charging tank g.
$XL_{v,t}$	Binary variable that denotes that vessel v starts unloading at time t
$XF_{v,t}$	Binary variable that denotes that vessel v finishes unloading at time t

Production and Product Blending Subsystem

dp	Depot
cm	Mixed crude into the CDU
t, T	Time interval for the planning horizon
g	All commodities
$intm\ (g)$	Intermediate materials from process units
$pmat\ (intm)$	Purchased material which include butane
FP, fp	Final products
$blnposs(fp, intm)$:	Blending possibilities

q, Q	Attributes for quality
u, U:	Process Units
$limits, lim$:	Upper and lower limits
$IP_{u,f,f',cm}$	Coefficient of yield from unit u based on feed stream flow rate f and output stream f' that depends on the type of crude mix cm
$IP_{u,intm,cm}$	Coefficient of intermediate product flow streams intm, from unit u which depends on the type of crude mix cm
$\mathrm{prop}_{\_\mathrm{fp}_{\mathrm{intm,cm,q}}}$	Attribute for blending the intermediate products
$\mathrm{propMAXFP}_{\mathrm{fp,q}}$	Maximum final product specification
$\mathrm{propMINFP}_{\mathrm{fp,q}}$	Minimum final products specifications
$\mathrm{BLINT}_{\mathrm{cm,intm,fp,t}}$	Level of intermediate material intm from crude mix cm that blended into final product fp during time period t
$Cost_{pr}$	Cost of refinery processes
$Cost1_{cm,t}$	Cost of crude mix cm during time period t
Cap_u	Capacity of process units
$Cost2_{pm,t}$	Cost of purchased material pm during time period t
COR_t	Cost of refining or refinery operations at time period t
REV_t	Total sales revenue from final products at time period t
RV_{fp}	Sales revenue from final products
$IMPCST_t$	Raw material cost at time period t
$\mathrm{FFP}_{\mathrm{fp}}$	Flow of final product fp
$PROLEV_{u,cm,t}$	Level of process u from crude mix cm at time period t
$PC_{cm,t}$	Purchased crude mix entering the unit (CDU)
X_i	Flow of intermediates from process units

$FM_{pm,cm,t}$	Flow rate of purchased material
RM_{fp}	Maximum production requirement
	Products distribution
CTR_t	Total Transportation cost for final products to depot at time t
$CINVPT_t$	Total Product tanks inventory cost
$\mathrm{V9}_{\mathrm{fp,pt,t}}$	Volume of final product fp from product tank pt to depot dp at time t
$\mathrm{cinv3}_{\mathrm{pt}}$	Inventory of final product tank pt
$\mathrm{V9}_{\mathrm{fp,pt,t}}$	Volume of final product fp from product tank to depot dp at time t
$\mathrm{vmax}_{\mathrm{pt}}$	Maximum volume of product tank pt
$\mathrm{vmin}_{\mathrm{pt}}$	Minimum volume of product tank pt
$\mathrm{F8}_{\mathrm{fp,pt,dp,t}}$	Flow of final product fp from product tank to depot dp at time t
$\mathrm{DEM1}_{\mathrm{fp,pt,dp,t}}$	Demand of final product fp from product tank pt at the depot dp at time t
$\mathrm{F9}_{\mathrm{fp,pt,t}}$	Flow of final product fp to product tank pt at time t
$\mathrm{V04}_{\mathrm{fp,pt}}$	Initial volume of product fp in the product tank pt at time t
$\mathrm{VFPDP}_{\mathrm{dp,t}}$	Volume of final product fp at the depot dp at time t
$\mathrm{VIDP}_{\mathrm{dp}}$	Initial volume of final product fp at the depot dp at time t
$\mathrm{CT}_{\mathrm{fp}}$	Transport cost for final products to depot at time t

1 Introduction

1.1 Introduction to refinery

The quest to develop the petroleum refining industry came from several changes in life-styles. The increased needs for illuminants, for fuel to drive the factories of the industrial revolution, for gasoline to power the automobiles, as well as the demand for aviation fuel, all contributed to the increased use of petroleum. The world prediction is that oil consumption will increase from 77.1 million barrels/day in 2001 to 118.8 million barrels/day in 2025 (Li, 2004).

A refinery is essentially a group of chemical engineering unit processes and unit operations for the purpose of converting crude oil into products of value while considering the qualities and quantities stipulated by the market (Tung-Hsiung and Chuei-Tin, 2008).

Figure 1-1 is a typical refinery topology, which is made up of the storage tank farm (e.g. storage tanks for crude oils, storage tanks for intermediate products, charging tanks) and the processing plants which is the most complex part of the refinery.

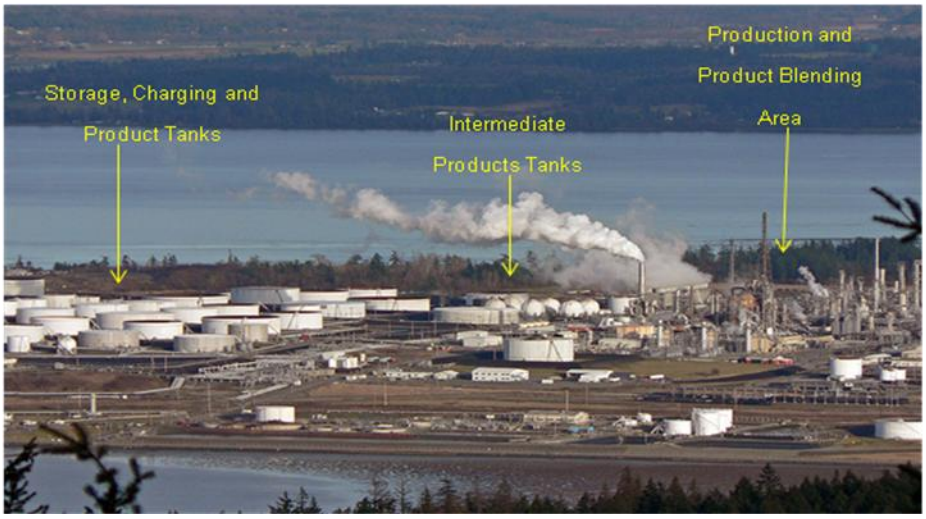

Figure 1-1 Topology of a Typical Refinery (Courtesy of the Standard oil company)

The refinery can roughly be divided into three main subsystems as shown in Figure 1-2, where C_i, P_i and DP_i *are* crude oil types, final products and depot or gas stations:

- Crude oil unloading subsystem
- Production and product blending subsystem
- Product distribution subsystem

Crude oils arrives in either a tanker, vessels or a truck and are stored in storage tanks for charging or blending before being refined and blended to meet the target set by the planners. These blended final products are then sent to depots or gas stations for retailing.

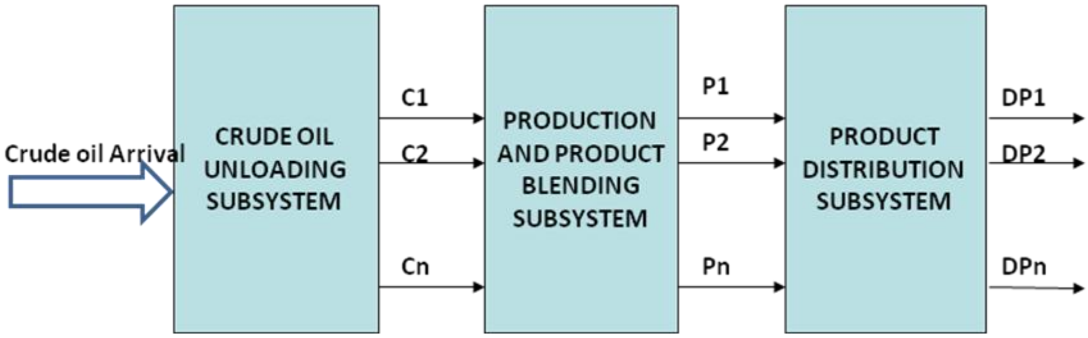

Figure1-2 Three Main Subsystems of a Refinery

1.1.1 Crude oil unloading subsystem

The crude oil unloading subsystem consists of unloading berths or docking stations, storage tanks, and charging tanks with pipelines connecting them. In some situations this subsystem is located near the sea for ease of loading and or unloading into the tanks for storage as shown in Figure 1-3. As tankers or vessels arrive at the refinery's docking stations/berths for unloading, the refinery ensures that there is sufficient capacity for storage.

Figure1-3 Crude oil Unloading Subsystem View

The Coryton refinery located in Essex on the Thames Estuary, southeast UK

Image courtesy of Terry Joyce (Courtesy ofHydrocarbonstechnology.com)

In the crude oil unloading subsystem of a refinery, various types of crude oil are purchased and processed. These crude oils are distinguished by their various compositions (Wu et al., 2006). The processing flow scheme of a refinery is largely determined by the composition of the crude oil and the chosen cuts of the petroleum products (Trzupek, 2002).

The compositions of processed crude have great influence on refinery margins. This gave rise to control of the quality of charged crude by refiners and the use of advance technologies to plan and schedule crude oil changes (Reddy et al., 2004).

1.1.2 Production and product blending subsystem

The production and product blending subsystem of the refinery consists of the Crude Distillation Unit (CDU), Vacuum Distillation Unit (VDU), Fluid Catalytic Cracker (FCC) and the Hydrotreater (HDT) units and other process units used to convert the crude to more valuable products. A view of the production and products blending subsystem is shown in Figure 1-4.

Figure1-4 A view of the Production and products blending subsystem vi

(Courtesy of Building green dot com)

Figure 1-5 shows the general processing arrangement of the production and product blending subsystem of a refinery. The design of a refinery is tailored to a particular crude oil specifications or properties; however, there are some basic process operations that are carried out in most refineries. Some of these processes are.

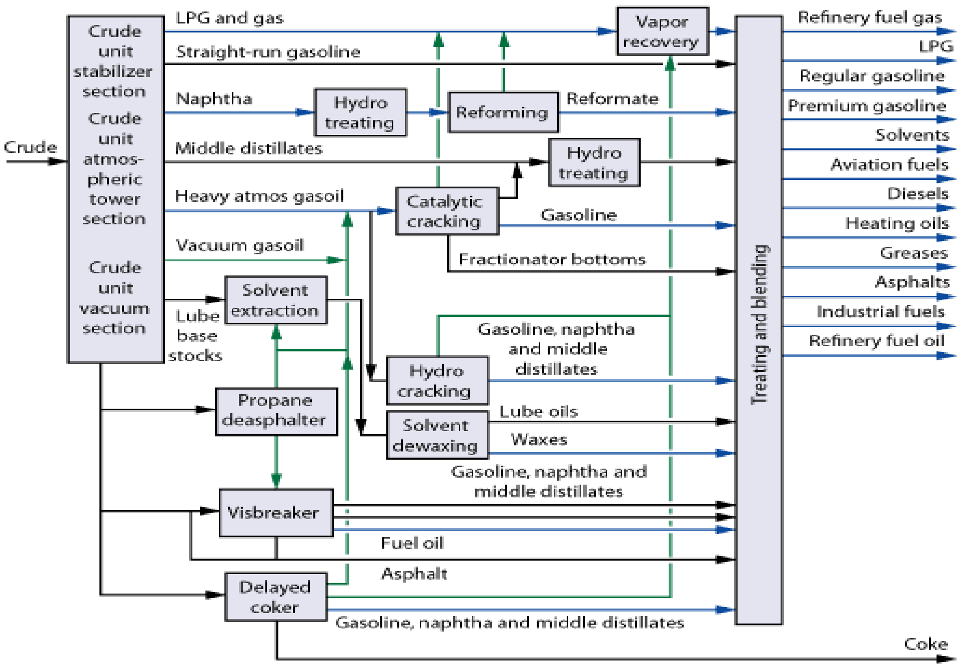

Figure 1-5 Complete activities of what happens in a typical refinery (Hydrocarbon processing, 2012).

1.1.2.1 Atmospheric tower or Crude Distillation Unit (CDU)

The crude is heated in a furnace and charged to an atmospheric distillation tower, where it is separated into butanes and lighter wet gas, unstabilized full-range gasoline, heavy naphtha, kerosene, heavy gas oil, and topped crude. The topped crude or atmospheric residue from the bottom of the CDU is sent to the vacuum tower and separated into a vacuum gas oil, overhead stream and reduced crude bottoms (Gary and Handwerk, 1975).

1.1.2.2 VDU

The feed into the VDU is the atmospheric residue from the CDU. The stream into the VDU is treated in the same way as the CDU but under high pressure. This VDU helps to further remove the distillate from the crude oil before being sent to the catalytic cracker unit. The reduced crude bottoms from the vacuum tower called the vacuum residue, is thermally cracked in a delayed coker to produce wet gas, coker gasoline, gas oil, and coke.

1.1.2.3 Catalytic processes

These are the conversion operations that further process the heavy and less valuable products from the distillation unit into high octane products. There are two types of such processes in refinery which are: Fluid Catalytic Cracking Unit (FCCU) and Catalytic Reforming unit (CRU) (Al-Qahtani and Elkamel, 2010). The atmospheric and vacuum crude unit gas oils and coker gas oils are used as feedstocks for the catalytic cracking or hydrocracking units.

1.1.2.4 Reformer unit

The gasoline streams from the crude tower, coker, and cracking units are fed to the catalytic reformer to improve their octane numbers. The products from the catalytic reformer are blended into regular and premium gasoline for sale.

The wet gas streams from the crude unit, coker, and cracking units are fractionated in the vapour recovery section into fuel gas, liquefied petroleum gas (LPG), unsaturated hydrocarbons (propylene, butylene, and pentenes), normal butane and iso-butane. The fuel gas is burned in refinery furnaces and the normal butane is blended into gasoline or LPG. The unsaturated hydrocarbons and iso-butane are sent to the alkylation unit for processing (Gary and Handwerk, 1975).

1.1.2.5 Hydro treating Process

Contaminants in liquids petroleum products are removed by means of hydro treating operations. The major concern is the presence of sulphur, nitrogen, oxygen and heavy metals in products distillation such as kerosene, naphtha, and diesel on which if not removed, will cause deactivation of catalyst and the yield of products which will fall short of environmental standards. The bottoms from CDU are also hydro treated before being fed in to the FCC unit in hydrodesulphurization process (HDS). Operating principle employed is hydrogenation reaction which takes place by reacting hydrogen with the feed at high temperature to form H_2S, NH_3, and H_2O. Generally, the nature of the feed and the level of treatment required determine the operating condition of hydro treating process. Treated liquid naphtha is separated and stabilized in a column to strip off H2S and light gases before being fed to CRU (Al-Qahtani and Elkamel, 2010).

1.1.2.6 Alkylation unit

The alkylation unit uses either sulphuric or hydrofluoric acid as catalyst to react olefins with iso-butane to form iso-paraffins boiling in the gasoline range. The product is called alkylate, and is a high-octane product blended into premium motor gasoline and aviation gasoline.

The middle distillates from the crude unit, coker, and cracking units are blended into diesel and jet fuels and furnace oils.

In some refineries, the heavy vacuum gas oil and reduced crude from paraffinic or naphthenic base crude oils are processed into lubricating oils. After removing the asphaltenes in a propane deasphaltene unit, the reduced crude bottoms are processed in a block operation with the heavy vacuum gas oils to produce lube-oil base stocks.

The heavy vacuum gas oils and de-asphalted stocks are first solvent-extracted to remove the heavy aromatic compounds and are de-waxed to improve the pour point. They are then treated with special clays to improve their colour and stability before being blended into lubricating oils.

Each refinery has its own unique processing scheme which is determined by the equipment available, operating costs, and product demand. The optimum flow pattern of any refinery is dictated by economic considerations and no two refineries are identical in their operation (Gary and Handwerk, 1975). Few if any refinery carry out all of these processes.

1.1.3 Product distribution subsystem

After the final products are produced, they are stored in the product tanks awaiting to be distributed to the various regions or depots that are located close to the consumers or retailers. The primary means of this transportation are ships, pipeline and rails while the secondary means are trucks as shown in Figure 1-6. In this thesis, trucks are assumed for transportation of the finished products to depots.

Figure 1-6 Product distribution subsystem view (Courtesy of Pacific L.A. marine terminal LLC, 2012)

1.2 Refinery planning

Planning is concerned with making available an adequate manufacturing capacity for broad classes of products (Edgar et al., 2001). Planning activities involves optimization of raw material supply, refining and subsequent commercialization of final products over one or several time periods (Pinto et al., 2000).A product is any item that the selection and quantity to be manufactured or produced is decided by top management (Alonso-Ayuso et al., 2005). In contrast, Scheduling is centred on details of material flow, manufacturing and production. Planning is forecast driven while scheduling is order driven.

Time horizon is the set of time periods within which planning is targeted (Alonso-Ayuso et al., 2005).The characteristics of planning is the time horizon of months or weeks, whereas scheduling tends to be of shorter duration, that is, weeks, days or hours depending on the cycle time from raw materials to final product (Edgar et al., 2001). Planning can be classified as follows (Kong, 2002):

- Strategic (long term) planning
- Tactical (medium term) planning
- Operational (short term) planning

1.2.1 Strategic (long-term) planning

This has to do with the decision on production network, plant sizing, product selection and product allocation among plants. It is also linked closely to a company's strategic business plan and direction. The objective is maximization of the expected benefit given by the net profit along the time horizon (Kong, 2002).

1.2.2 Tactical (medium-term) planning

This is concerned with deciding on the best utilization of limited or available resources including vendor, factories, depots, and dealer centres along the time horizon such that given targets are met at a minimum cost or profit maximized (Kong, 2002).

1.2.3 Operational (short-term) planning

This is concerned with determining operations assignment to process plant and also the sequencing and scheduling of jobs and operations along a time horizon, given a production network, a specific job demand and operations target (Alonso-Ayuso et al., 2005). This is subject to the constraints in current inventory of crudes, blending feedstock and a set of forecasted crude deliveries. The updates are at regular intervals e.g. monthly, weekly or in response to changes in level of inventory, receipt of any changes in raw material delivery schedule or sudden changes in the style of demand. Short-term or operational planning is called scheduling at the production stage (Kong, 2002).

1.3 Refinery scheduling

Oil refineries are increasingly concerned with improving the scheduling of their operation (Pinto et al., 2000). In the refinery supply chain, crude oil scheduling is vital.

Efficient crude scheduling manages plant shutdown, excessive flaring, demurrages and stock-out (Hartmann, 1997). It also determines the type of blending recipe to use that satisfies planners' quantity and quality targets.

In crude oil scheduling operations, the decision makers are faced with factors concerning the vessels arrival time, the unloading of the vessels, the time for brine and water to settle and the charging of the CDU with the crude oil. Handling this manually could be complicated and inefficient as these conditions changes all the time. It will not also guarantee that the operation is carried out at minimal cost and hence a scheduling model is necessitated.

Planning and scheduling can be summarised as follows in Table 1-1: (Edgar et al., 2001).

Table 1-1 Difference between planning and scheduling

planning	scheduling
• tactical	• operational
• aggregate data	• detailed data
• describe large segments of production environment	• describe smaller segments
• planning horizon: months or weeks	• planning horizon of few hours to several days/weeks

1.4 Motivations for the study

Due to the increasing demand for petroleum products, the cost of crude oil and the set environmental regulations need to be observed and monitored strictly, tools required for production planning and management decision making become inevitable for the refinery economic evaluation (Guyonnet et al., 2009).

In modern refineries, the planning department is relied upon for decision making such as final product demand forecasting, crude oil procurement, production and product blending and product distribution.

1.4.1 Modelling for refinery planning

Experience has shown that it is more practical and profitable to use mathematical models for the purpose of planning (Wagner, 1975). This has been encouraged due to initial successes recorded, and has also pioneered linear optimization methods to a wide variety of decision areas, which led to the demonstration of techniques for making this scientific approach realizable in a competitive business environment (Wagner, 1975).

There are many mathematical programming models that exist on refinery planning. For proper model development and selection of suitable mathematical modelling techniques good understanding of the process interactions, experience and practice is required (Al-Qahtani and El-kamel, 2010).

Refinery planning models are mostly linear. However, non-linearity can arise which is mainly associated with product yields from the refinery units, blending and the pooling of intermediate product.

1.4.2 Modelling for production planning

In the production and products blending subsystem of the refinery, the refining area is the place where most of the production activities are performed, activities such as converting crude oil into more valuable products, to meet customers demand and quality specifications. The profitability of a refinery will be maximized if these operations are run as efficiently as possible. There has been so much argument on the accuracy of using linear model for CDU, VDU, FCC unit and HDT unit in refinery planning. Refining processes are nonlinear (Slaback, 2004), but the tabulated values of yield and quality of intermediates products produced are linearized and used in an optimization planning model (Brooks and Walsem, 1999).The results obtained from using rigorous models for processing units are more accurate (Li et al. ,2005).

1.4.3 Refinery planning for crude oil mix

Refining of crude oil blends is increasing due to the increase in crude oil price, meeting stringent regulations, making profit and the need to meet the demand of petroleum products that has been programmed for the refinery. This has resulted in most refiners buying different crude oil (sweet or sour, heavy or light) and blending them to meet the processing unit specifications. Accurate modelling to obtain information on yields from these units for refinery planning is essential.

In the past, several methods have been developed for modelling CDU and VDU to obtain information on product yields and then used for refinery production planning.

The major challenge faced by refiners is to enhance the distillate yields by optimizing the mixed crude oil to make them profitable (Shaoping et al., 2010). The cost of crude accounts for about 80% of the refinery expenditures, which means that when cheaper crude is processed, it has a positive impact on the refinery profit margins (Stratiev et al., 2010).

1.4.4 Planning for the integrated refinery subsystems

Planning and scheduling models for refineries should look at modelling each of this subsystems and realizing the material flow by the integration of all subsystems (Li, 2004).

An integrated modelling approach would provide a better link between the main subsystems of the refinery, and management of inventory will be achieved while resolving the issues between the crude oil supplies.

Recent advances to enhance refinery planning model have centred on proper integration of models i.e. integrating the three main subsystems with the refinery planning and the idea of integrating multiple refineries for proper production management (Guyonnet et al., 2009).

Some researchers gave an extensive review on the integration of models on production and product planning and product distribution model. The reason is that, this integration could be achieved by feeding the crude oil unloading subsystem by information from production and product planning or vice versa as in Figure 1-7and their conclusion is that a heuristic based Lagrangian decomposition could be used for the integration. In spite of the arguments, no integrated model exists for the planning of the three subsystems (Guyonnet et al., 2009).

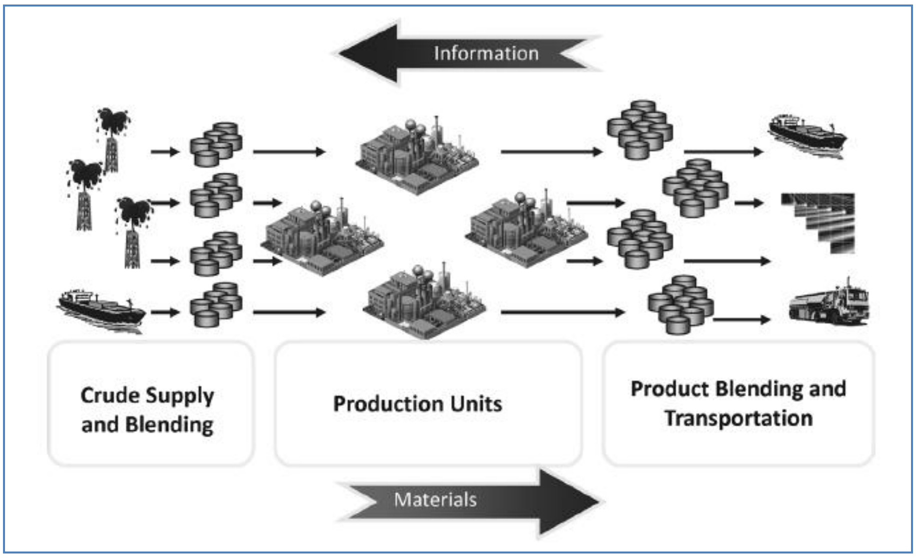

Figure 1-7 Schematic showing information and material flow in integrated system

1.5 Research aim, objectives and Scope

This thesis is aimed to deal with tactical (medium term) planning for the integrated refinery subsystems using Mixed Integer Linear Programming (MILP). The following objectives are meant to be achieved:

- To develop a rigorous model for CDU and VDU. Validate the model and analyse.
- To develop an aggregate planning model for the processing units for refinery planning for the production and product blending subsystems.
- To carry out a case study with the aggregate model and implement using mathematical programming.
- To modify a short term MILP scheduling model by Lee et al. (1996).
- To integrate the developed aggregate mathematical planning model with crude oil unloading subsystem model, and product distribution subsystem model and implement in under deterministic condition in refinery planning implement in GAMS.
- To carrying out Case studies from a refinery in West Africa to demonstrate the applicability of the proposed model and solution approach.

The scope of this research: In this work, two different types of crude were considered namely: Brent and Ratawi crude. The crude property considered is the sulphur content in crude oil mix. This is because the sulphur content of crude affects the price of the crude and the profit margin of the refinery. Only LP and MILP were investigated for refinery planning. NLP or MINLP were not studied in this thesis since the relationship between the product yields and the sulphur content in the crude mix was found to be linear.

1.6 Methodology

Figure 1-8 is used to illustrate the methodology used to achieve the set objectives in this work.

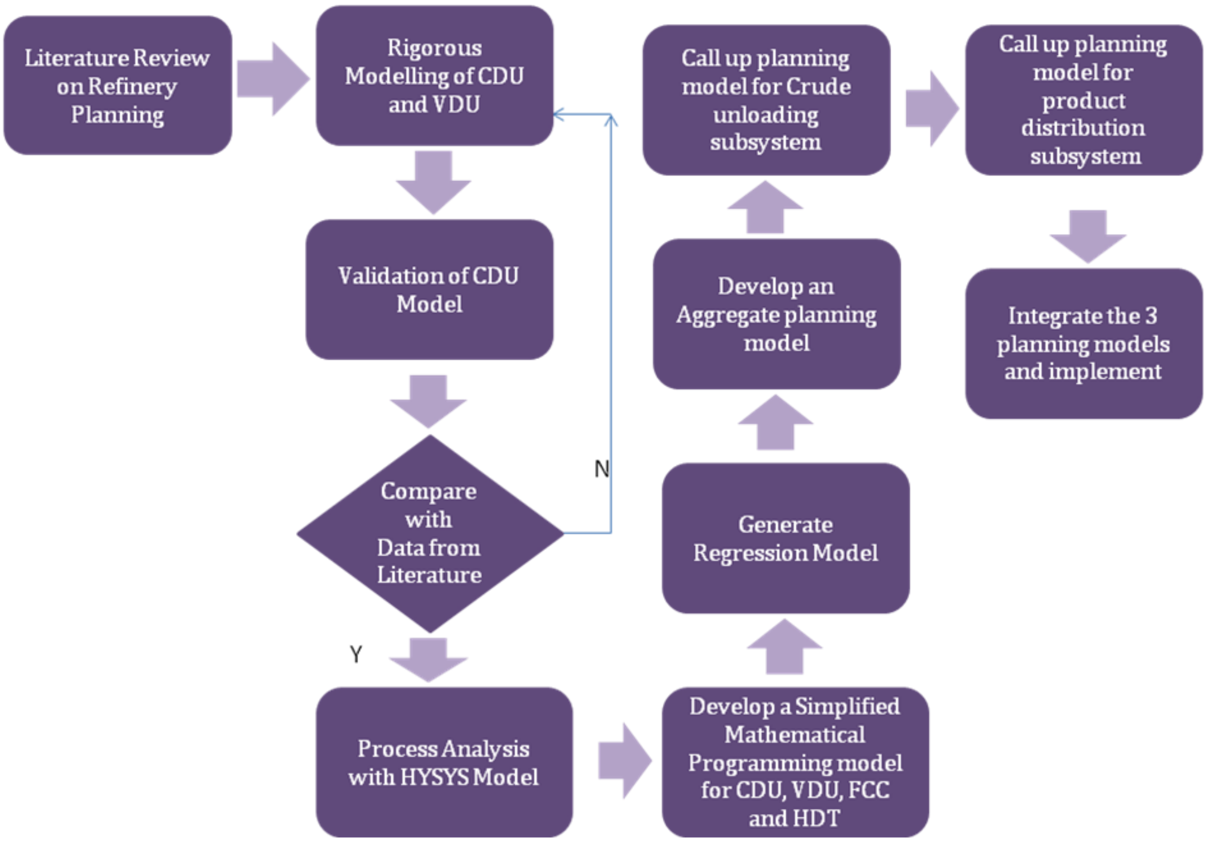

Figure1-8 Overview of research methodology

1.7 Novelties in this thesis

- Use of mixed crude rather than the single crude generally used for refinery planning models.

- Development of a rigorous model for CDU and VDU and information transfer from the rigorous model for CDU and VDU into simplified CDU and VDU model for planning.
- Development of an aggregate model for planning of the production and product blending subsystem of a refinery.
- Integration of the aggregate model for production and product blending subsystem with modified scheduling model for crude oil unloading subsystem and products distribution subsystem for refinery planning.

1.8 Computational tools used

1.8.1 Introduction to GAMS

Substantial progress was made in the 1950s and 1960s with the development of algorithms and computer codes to solve large mathematical programming problems. The number of applications with these tools in the 1970s was less than expected, however, because the solution procedures formed only a small part of the overall modelling effort. A large part of the time required to develop a model involved data preparation and transformation and report preparation. Each model required many hours of analyst and programming time to organize the data and write the programs that would transform the data into the form required by the mathematical programming optimizers. Furthermore, it was difficult to detect and eliminate errors because the programs that performed the data operations were only accessible to the specialist who wrote them and not to the analysts in charge of the project (Brooks et al., 1997).

GAMS was developed to improve on this situation by:

- Providing a high-level language for the compact representation of large and complex models
- Allowing changes to be made in model specifications simply and safely
- Allowing unambiguous statements of algebraic relationships
- Permitting model descriptions that are independent of solution algorithms.

GAMS which represent general algebraic modelling system is specifically designed for modelling linear, nonlinear and mixed integer optimization problems. The system is especially useful with large, complex problems. GAMS is available for use on personal computers, workstations, mainframes and supercomputers. GAMS allows the user to concentrate on the modelling the application problem by making the setup simple. The system takes care of the time-consuming details of the specific machine and system software implementation (Brooks et al., 1997).

1.8.2 Introduction to Aspen HYSYS®

Aspen HYSYS® is used to create rigorous steady state and dynamic models for plant design, performance monitoring, troubleshooting, and operational improvement and asset management in process industries.

The reasons for choosing Aspen HYSYS are as follows:

- Aspen HYSYS provides the accuracy, speed and efficiency required for process design activities.
- The level of detail and the integrated utilities available in Aspen HYSYS allows for skilful evaluation of design alternatives, with fast and efficient process simulation.
- It is an interactive, project-oriented programme.
- It has the facility for interactively interpreting commands, as they are entered one at a time (Seider et al., 1998).

1.9 Outline of the thesis

Chapter 2 will review current practice on planning of the individual subsystem, integrated subsystems under deterministic condition.

Chapter 3 will focus on developing a rigorous model for CDU and VDU. The model will be validated with pilot plant data from literature and further analysed.

The information from the rigorous modelling is used to develop a simplified mathematical programming planning model and implement in a refinery production and product blending subsystem planning model in Chapter 4. Empirical correlation by Gary and Handwerk (2001) is used for the FCC and HDT units with consideration of the crude characterization, products yields and qualities. 53 scenarios or volumetric mixing ratios from Aspen HYSYS model is carried out to determine the volumetric ratios that gives the highest profit.

In chapter 5, an aggregate model for predicting the yield from CDU and VDU is developed, validated and applied in refinery production and products blending planning. The developed model is applied to a case which is used for comparison with the regular fixed yield counterpart.

Chapter 6 will detail on the integration of the modified crude unloading subsystem model, the developed aggregate model in chapter 4 and already existing products distribution planning model. The model for the three subsystems shall be applied to a case study for the planning of a refinery. This refinery planning model is based on deterministic approach.

Chapter 7 will then be conclusions and recommendations for future works.

2 Literature Review

2.1 Introduction

In this chapter, the techniques used for mathematical optimization and the benefits of using LP are described. Planning in oil refineries and recent practice in modelling process units for planning in oil refinery is reviewed. The review will also cover scheduling and its models for the refinery, and recent advances in refinery scheduling. Finally, the integration of planning and scheduling model is reviewed. The future trend for refinery planning is included.

2.2 Mathematical optimization techniques

Optimization makes use of efficient quantitative method to select the best among the entire set of solutions. The aim of optimization is to determine the values of the variables in the process that yield the best value of the performance criterion (Kallrath and Wilson, 1997).

Usually a mathematical programming model in optimization consists of four key objects

- Objective function
- Decision Variables (continuous, semi-continuous, binary, integer)
- Constraints(equalities, inequalities), and
- Parameters.

Mostly, objective function focuses on either maximising the profit that is generated for a particular plan, or minimizing operational cost for scheduling, blending and transportation subject to constraints that describes the operating conditions (Kallrath and Wilson, 1997). Identifying the possible decisions or problem variables to be made is the first step taken in any decision problems. Next is to identify the decisions that are admissible which leads you to the set of constraints that needs to be determined according to the nature of the problem in question. The information or values available are called the parameters (Enrique et al., 2002).

In the past, manual calculations were used in solving optimization problems for industries and other establishment with inaccuracies existing in the solutions and time consuming factors. This progressively changed to the use of spreadsheet which has proven to be more accurate and less rigorous compared to the manual calculation. But the use of mathematical programming and different applications has long taken over the petroleum industry. The invention of both the simplex algorithm and digital computers was what propelled the spread of LP applications in the industry followed by many other applications in the area of refinery planning (Al-Qatahni and Elkamel, 2010).

When developing refinery mathematical optimization models, they usually lead to structured problems such as

- LP problems
- Nonlinear programming (NLP) problems
- Mixed Integer Linear Programming (MILP) problems
- Mixed Integer Non-Linear Programming (MINLP) problems.

2.2.1 LP

LP involves problems in which both the objective function and the constraints are linear. The word programming in this context means optimization. It is the most widely used optimization techniques. For example,

$$\max \quad 2x + 4y + 3z \tag{2-1}$$

$$Subjectto: 3x + 2y + z \leq 38.5 \tag{2-2}$$

$$x + y + 1.3z = 10.0 \tag{2-3}$$

$$4y - z \quad \geq 6.2 \tag{2-4}$$

$$x, y, z \geq 0 \tag{2-5}$$

Equation (2-1) represents the objective function, Equation (2-2), (2-3), (2-4) and (2-5) are the constraints while x, y and z are the variables.

The features of LP problems for these examples are:

- There is an objective function which is to be maximized. There is no multiplication of variables such as x*y or introduction of mathematical functions such as power, exponential, trigonometric functions of variables generally. It is the objective function which drives the process of optimization.
- The constraints are also linear in expressions on the left hand side. They are linked to a constant at the right hand side by a relation which will be one either of $\geq, \leq$ *or* $\equiv$. No other relations are permitted.
- There is also a requirement that the variables cannot take negative values.
- In the linear expressions the constants are usually rational real values, whole numbers and decimal fractions are included but not expressions such as pi or roots, which can only be included by approximating them to a given number of digits.
- Inequalities $<$ or $>$ are not permitted in the constraints, but this turns out not to be a drawback. Usually practical models will only require $\geq$ *or* $\leq$ constraints

  (Kallrath and Wilson, 1997).

Limitations of LP programming techniques

- LP can only handle a single objective which may be unsatisfactory
- In the constraints and objective function of an LP problem, the assumption has to be made that all modeling can be made linear.

Advantages of LP programming techniques

Problems associated with process that are inherently nonlinear are simplified when modeled with LP i.e. products properties and feed variance as well as changes in process conditions of operation and their relationship. LP provides a reliable value structure especially the issue of marginal prices for products.

In solving optimization problems in refinery planning, LP approach is mostly preferred to other optimization algorithm due to its convenience (Zhang and Zhu, 2006).

The ease of formulation of LP problems and its use for approximating nonlinear model around its steady state made it a preferred tool. Since LP model is one of the oldest techniques for optimization, it has been widely applied in the area of planning for manufacturing and processing industries for obtaining global optimum and reliable solutions. Hence there is vast information and experiences on LP which is readily available; this made LP an easy alternative for planners to make use of. Also, the simplified, robustness and fast nature of the solution time of LP in comparison with other techniques makes it a quick decision making tool when profit is the ultimate focus.

Operationally, LP establishes operating strategies and goals of real operations. In as much as the choice for LP is a tradeoff between simplicity and robustness with accuracy of the solution obtained especially when nonlinear processes are approximated, the solutions obtained are optimum with accurate data. LP provides the means of interpreting the optimum results in simple and concise manner for better understanding in many industries for better grasp of business or industrial problem (Simon and Azma, 1983).

Finally, most of the existing commercial software for refinery production planning such as RPMS (Refinery and Petrochemical Modeling System) is based on a very simple LP model which mainly is composed of linear relationships (Pinto et al., 2000).

2.2.2 NLP

This is a programming problem with some nonlinear constraints, or a nonlinear objective function, or both. It can be represented with the following equation:

$$minimise: f(x) \tag{2-6}$$

$$Subjectto: ai \leq gi(x) \leq bi \qquad (2\text{-}7)$$

$$lj \leq xj \leq uj \qquad (2\text{-}8)$$

$wherei = 1, \dots .., mandj = 1, \dots \dots, n$ (Edgar et al., 2001)

Equation (2-6) is the objective function, while Equation (2-7) and (2-8) are the constraints.

Due to the fact that refinery operations exhibit some inherent non-linear characteristics when modelled, they are often approximated into linear models for simplicity and ease of computation. NLP model was developed by Moro et al. (1998) for planning of the entire refinery with all the process units represented and non-linear blending relations.

Pinto and Moro (2000) presented a nonlinear model for each unit and the combination of the whole refinery. Neiro and Pinto (2004) transformed the same model framework into a multi-period and multi-scenario model in their attempt to generate models that truly covers and represents all the features of a refinery.

Companies are developing in-house commercial software packages for NLP models but are faced with challenges of convexities and difficulty of convergence which is the reason why NLP are often referred to as 'NP hard', hence, the industries are ultimately left with the option of LP based software for solving their refining planning models. Though, some achievement are made in building NLP models but it has short comings of the solution being local and specific to a particular plant and situation which makes it difficult for bench marking for global solution (Alattas, et al., 2011).

2.2.3 MILP

When an LP contains integer variables, or certain other type of variables, it becomes an MILP problem, usually containing both integer and continuous variables.

MILP retains the linear objective and constraints but adds an integrality attribute to the non-negativity requirement on some, or all of the variables. Models that can be formulated using MILP contains the following features and properties,

- Counting
- Representation of states and yes –no decisions
- Logical implications
- Simple non-linear functions

For example:

$$\max z = 3c + 2p \tag{2-8}$$

$$Subject\ to: \qquad 0 \leq c \leq 2 \tag{2-9}$$

$$0 \leq p \leq 2 \tag{2-10}$$

$$c + p \leq 3.5 \tag{2-11}$$

where c and p are integer (Kallrath and Wilson, 1997)

Advantages and Limitations of MILP

One of the advantages of MILP approach is that it provides a general framework for modeling a large variety of problems such as multi-period planning, job shop scheduling and supply chain management problems.

However, the major difficulty lies in the computational expenses that may be involved in solving large scale problems, which is due to the computational complexity of MILP problems which are non-deterministic polynomial time hard (NP-hard).

2.2.4 MINLP

A technique to solve optimization problems which allows some of the variables to take on binary, integer, semi-continuous or partial integer values, and allows nonlinear constraints and/or objective functions (Kallrath and Wilson, 1997).

2.3 Planning in oil refineries

Petroleum refineries are increasingly concerned with the improvement of their planning operations (Pinto et al., 2000).Well developed, fairly standard and widely understood tools and technologies are used for refinery planning. However, evolutionary changes are expected e.g. refinery models need to be more accurate and improved by the combination of rigorous model runs plant test, vendor data e. t. c. (Pelham and Harris, 1996).

Applications of planning models in the refinery and oil industry include crude selection, crude allocation for multiple refinery situations, and partnership model for negotiating raw material supply and operations planning. And with appropriate planning, new technologies for process operations can be integrated for profitability.

Due to increase in scope and size of optimization problems over the years, refiners are forced to engage the services of optimization software for quick and efficient solution for profit maximization. Activities in planning involve optimization of raw material supply, processing and subsequent commercialization of final products over one or several time periods (Pinto et al., 2000).

The commercial software packages, such as Refinery and Petrochemical Modeling System (RPMS) (Shah et al., 2011), *General Algebraic Modeling System* (*GAMS)*, Process Industry Modeling System (PIMS) (Zhang and Zhu, 2006), Petroplan and host of others, are developed to solve the wide range of practical problems that arise in refineries.

RPMS is based on a very simple model which mainly is composed of linear relationships, the production plans generated by these tools are interpreted as general trends (Pinto et al., 2000). Li et al. (2005) presented a refinery planning model that utilizes simplified empirical nonlinear process models. He demonstrated how CDU, FCC and product blending models are formulated and applied to refinery planning. The refinery planning model was formulated in GAMS.

2.3.1 Types of planning models

There are two main types of planning models, these are:

- Rigorous models
- Empirical models

2.3.1.1 Rigorous models

These are models that are based on the theoretical understanding of the system and process variables interactions. Application of conservation principles are the bases of this method (i.e. energy and material balances) and equilibrium phase relationships. One of the major advantages of this model is the ability to formulate them before putting the system into operation (Al-Qatahni and Elkamel, 2010).

2.3.1.2 Empirical models

These are data driven models, also known as black box models. These models are found to be useful when rigorous models cannot be implemented due to limited resources or are found to be complex. In this type of planning model, the systems are seen in terms of inputs, outputs, and their relationships without any knowledge of the systems internal mechanism.

2.3.2 Modelling of process units for refinery planning

2.3.2.1 CDU

CDU is one of the major processing units in the refinery downstream operation. Two types of model are usually used in CDU modelling, namely; Empirical and Rigorous (Li, 2004).

Empirical models for CDU

Empirical models make use of empirical correlations to determine material and energy balances for CDU. It was initially proposed by Packie (1941), and Watkins (1979) expanded on it. These correlations are also very much ideal for preliminary design purposes (Li, 2004).

Rigorous models for CDU

Rigorous models simulate a CDU taking into account phase equilibrium, heat and mass balance all through the column. The advantage of such rigorous model includes results on flow rates, compositions of streams internally and externally and optimal operating conditions. Research work has continuously been carried out just to improve rigorous models.

Due to the challenges involved in rigorous modelling, people do work on numeric models. Some researchers applied the θ method of convergence in modelling of the main column to obtain a steady state solution that is equal to the field data (Huang, 2000). Other researchers like Hess et al. (1977) and Holland (1983) made use of 2N Newton -Raphson method on the tower for steady state solution. Russell (1983) implemented an 'inside out' approach to model a CDU, this method uses a combination an existing technique, which allows a very wide specification. Very little information is required at start and the speed of processing is better than other techniques.

Also commercially available software packages, such as Aspen Plus (Aspentech), PRO/II (SimSci-Esscor) and design IITM (ChemShare), have been developed and are commonly used. Rigorous simulation model has proven reliable and flexible since the steady state results can be matched with field data.

2.3.2.2 VDU

In crude oil distillation, one of the goals is to maximise the extraction of the distillate liquid from the raw crude. These distillates also called reduced crude sometimes serve as feedstock to other process or processes where values are added to the material. Crude distilled in the atmospheric tower still contains some more distillable oils that can be further distilled under vacuum. For 30 degree API crude, the vacuum distillates can get up to 30 percent volume of the whole crude. This justifies why refiners need to recover as much more distillates from given crude (Watkins, 1979).

2.3.2.3 FCC

FCC unit is another important process unit in a refinery. Currently, the ability of a refinery to be profitable in a competitive market also depends on the successful operation of the FCC unit (Slaback, 2004). 40 percent of the feedstock to the gasoline blending process is from the FCC (Lin, 1993). This implies that FCC unit model should be included in a detailed study of a refinery.

The purpose of the FCC unit is to breakdown the high-boiling, heavy components in the crude oil into lighter, more valuable products. Previously, thermal cracking was used to convert the heavy gas oil to lighter products. However, the catalytic cracking process has now replaced thermal cracking due to its ability to produce more gasoline with a higher octane rating (Gary and Handwerk, 2001). Zeolite catalyst is commonly used in FCC unit operations (Slaback 2004).

Pinto et al (2000) applied a linear model to FCC unit. On the other hand, due to the nonlinear nature of FCC, a linear model may not give reliable values on the yield and properties of FCC distillates (Li 2004). Some researchers like Guyonnet et al. (2009), Pongsakdi et al. (2006) and Neiro and Pinto (2005) used the same FCC unit model by Pinto et al (2000) may give inaccurate yield of the unit.

Methods have been developed by Gary and Handwerk (2001) to obtain the yields of FCC unit from simple feed properties and known conversion from charts and figures. These methods are useful for obtaining typical yields for preliminary studies (Li, 2004) and shall be implemented in this work.

2.3.2.4 HDT

Hydro treating is a process removing sulphur and or any objectionable elements from products or feedstock by reacting them with hydrogen to meet product specification (Gary and Handwerk, 2001).

The HDT receives feed from the CDU and VDU unit. To calculate the fraction of the products from the HDT, the correlation by Gary and Handwerk (2001) was implemented i.e. the product yield from the HDT is about 98 volume percent of the feed (Same boiling range as feed). Yields of light product were assumed (2 volume percent). This is due to the fact that very little literature on yields of HDT has been published.

2.3.3 Current methods for CDU modelling in refinery planning

CDU is one of the processing units that determine the profitability of the refinery. The raw material for other processes is generated in the CDU. The operation of the CDU is classified into modes, such as gasoline or diesel mode, which depends upon the properties of the crude, the process constraint etc. in each of this modes, there exist a set of predetermined cutpoints.

CDUs of a refinery can be modelled for planning purposes in different ways, including the product yields and property of the crude oil distillation in the planning model. The approaches reported include a fixed yield representation model, swing cut model (Li , 2004), and fractionation index (FI) Alattas et al. (2011). Most of these methods relied on the distillation behaviour of each crude oil pre-determined by crude assay outside and distillation simulation program where crude oil are cuts at designated temperatures and the resultant yields and properties information are passed to an LP model.

2.3.3.1 Fixed yield approach

Fixed yield method is one of the widely used methods for CDU modelling and it is the oldest method practised in most refineries. Though efforts has been made to improve or develop new ways of modelling the CDU. However, the resulting approaches have always resulted to fixed yield with nonlinear or more complex algorithm.

Fixed yield model is linear based approach that is employed for predicting yield. This approach uses rigorous or empirical models for the determination of the material and energy balance for the unit. In the fixed yield model, the cuts fractions as shown in Figure 2-1 at various designated temperature on the True Boiling Point (TBP) curve would be determined by the simulator based on the phase equilibrium, material and energy balances in the whole column under steady state using the crude assay and the result of the cuts and property information passed on to the LP planning model. Figure 2-2 describes the structure.

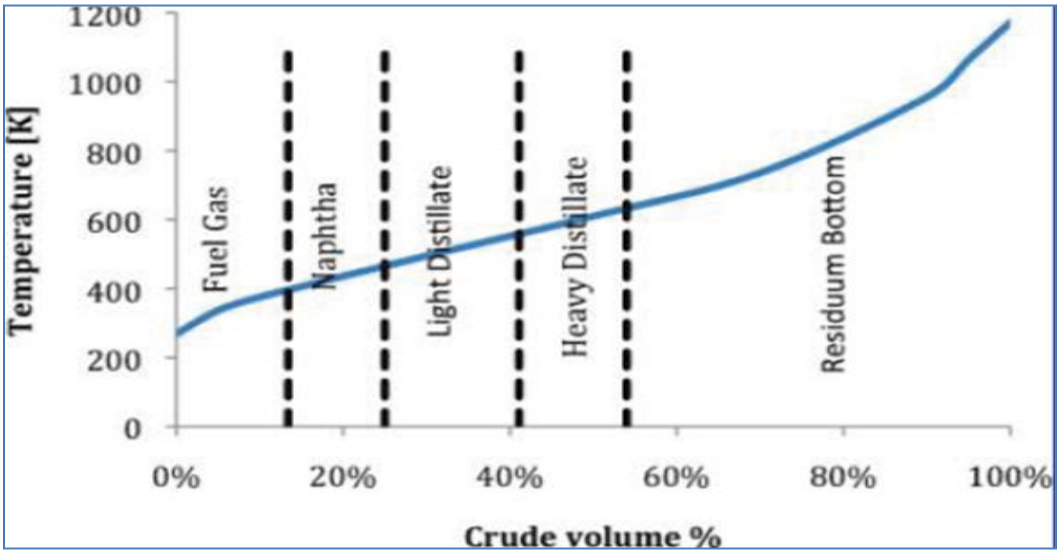

Figure 2-1 Fixed Yield Model (Adapted from Alattas et al. 2011)

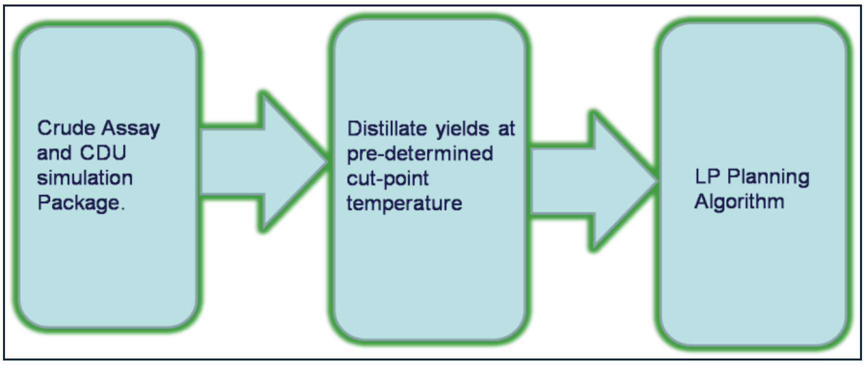

Figure 2-2 flow diagram of a Fixed yield structure representation

Some authors applied a method known as “Adherent Recursion” to optimize cut points. Here the result obtained from LP model (new cut points) were resent to the simulator for yields and property updated.

The fixed yield method is rigorous and simple and does not introduce non-convexity because it uses linear equation for CDU representation in the refinery planning model.

2.3.3.2 Swing cut method

In swing cut approach, physically non-existent cut are defined in the LP model. This is illustrated in Figure 2-3. GO (Gross overhead) and HN (Heavy Naphtha) are the two distillates of a CDU. For the LP to have the flexibility of adjusting the volume transfer ratio of the two distillates, two adjustable pseudo-cuts, shown as the two rectangles in

Figure 2-3 are added. The range of a swing cut is defined as a certain ratio on the crude feed bounded by limits, e.g. segment B-D defined the quantity of a cut (say 5% of the total fed crude) that could go to either of the two distillates. The final volume ratio of GO is depicted as segment A-C. In the same way, as soon as the HN swing cut is apportioned, the final volume transfer ratio HN can be shown as segment C-E (Li, 2004).

In swing cut approach, distillation behaviour is not accurately represented due to the non-linear nature of the distillate properties. Also swing cuts into adjacent draws are assumed to be linear whilst the actual property distribution in crude oil is highly non-linear.

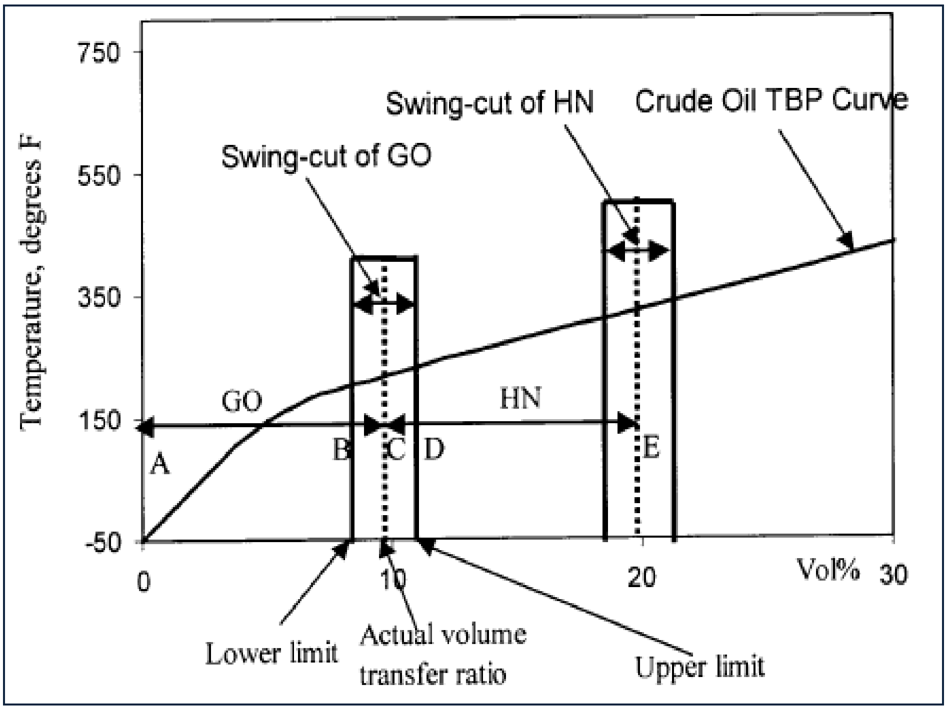

Figure 2-3 Swing cuts model (Reproduced from Li, 2004)

2.3.3.3 Fractionation-index method

Another practice is the Fractional Index (FI) method. In FI practice, the CDU is modelled as a series of fractionating units as shown in Figure 2-4. It uses the relative volatility of a component in relation to the top and bottom product streams in the CDU that is expressed as molar fraction. The top products are fed to the next unit while the bottom products are withdrawn as CDU products, except for the last unit where the top is withdrawn as overhead.

The FI method was initially proposed by Geddes, (1958) and subsequently Gilbert et al., (1966) extended it to CDU. Given the temperature ranges of the cuts, feed crude oil assay, feed rates and FI values, for each unit the total and component mass balance and the FI equation for the equilibrium calculation is applied.

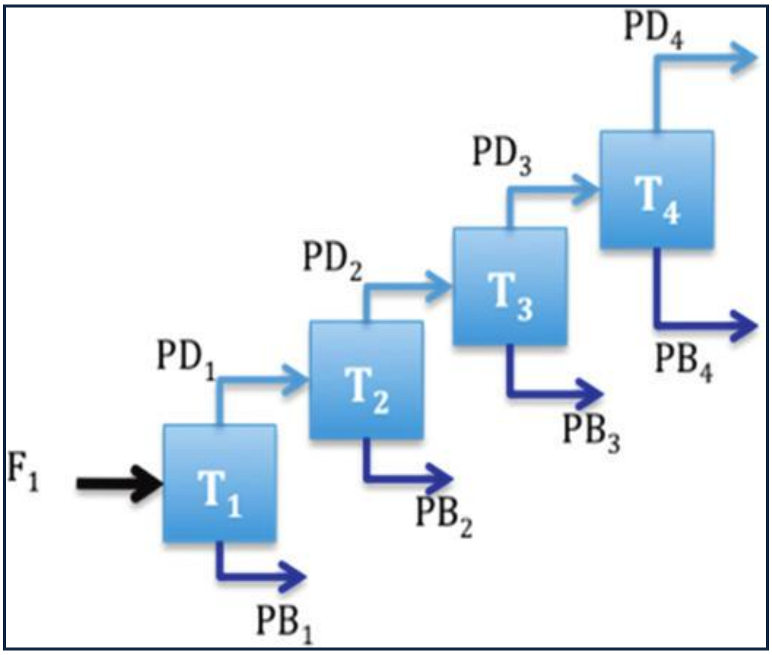

Figure 2-4 The FI model (Reproduced from Alattas et al., 2011)

In FI approach, the yield purity is jeopardized because the bottom product being collected as yield at a particular temperature T1 in PB1 may not have been completely condensed, so the temperature of the vapour going into the next stage may enter with entrained liquid of the bottom product. This method introduces non-convexities.

Recent advances in refinery planning

Due to increase in scope and size of optimization problems over the years, the solving of refinery problem has taken a new aspect as petroleum refiners engage in the use of software for quick solutions in an attempt to achieve maximum profit out of the available resources within a particular time horizon.

These software are used to simulate the processing units to generate operating conditions (e.g. temperature and pressure), yields and their properties to be optimized in an existing planning model. Some refineries and petrochemical industries modify or customise the simulators to solve problems based on their specific need. e.g. problems on production planning, supply chain planning, material requirement planning, blending, crude oil selection and evaluation, uncertainties in the operation environment and to forecast future trend and opportunities. In the design and planning of refinery processes to generate cuts which are further optimized, empirical correlations are used (Watkins, 1979)

2.3.3.4 Production and product blending subsystem

The production and product blending area of the refinery consists of the CDU, FCC, catalytic reformer (CR) and the HDT and other process units used to convert crude to a more valuable product while the products qualities such as sulphur, octane number, vapour pressure and product quantities are not compromised.

Usually the objectives of the individual units are conflicting and thus contribute to a sub-optimal and many times infeasible overall operation. Optimization of process units, online optimization of CDU has been carried out by Basak et al. (2002). Optimization of secondary processing units such as CC and hydrocracking units are also an area of importance due to the role it plays in the oil refinery. Lee et al. (1970) used dynamic programming to determine the operating condition in a CC that maximized the profit function.

Li et al., (2005) went further to integrate the CDU, FCC and product blending models into refinery planning. What they did was to develop a refinery planning model that utilizes simplified empirical linear process models with considerations on crude characteristics, product yields and qualities.

Planning models for production and products blending subsystems have been developed by Pinto et al. (2000), Moro et al. (1998), Joly et al. (2002), Nero and Pinto (2005), Li et al. (2004), Khor et al (2008), Alattas et al. (2011). Li et al. (2004) considered uncertainty in their model; they derived a loss function and applied it in calculating the expected plant revenues. Uncertainty was considered in crude supply and product demand. Pongsakdi et al. (2006) addressed the issue of uncertainty and the financial risk aspect for refinery operations. Jeongho et al. (2010) also considered financial risk management in refinery planning. In their work, they considered uncertainty in crude price and product price in the production and product subsystem of the refinery using LP. Chufu et al. (2008) developed a hybrid programming model for refinery production planning. In their work they considered uncertainty in product demand using LP.

Very little information is available in the published literature on overall optimization of oil refineries, but many studies have been reported on the optimization of process units. The optimization of the production units does not achieve the global economic optimization of the plant (Pinto et al., 2000), hence the need to integrate the refinery subsystems.

2.3.3.5 Integrated modelling approach for the subsystems

Since integrated modelling approach provides a better link between the three main subsystem of the refinery, Neiro and Pinto (2005) presented a nonlinear model for refinery planning which deals with the supply chain management for multiple refinery sites, they considered uncertainty in crude and product price as well as demand using scenario based approach with two time periods, however they did not consider crude oil operations and distribution in detail. Pitty et al. (2008) presented a dynamic model of refinery supply chain operation, they considered suppliers and customers, functional departments in the refinery, production units and refinery economics. However, their model did not provide explicit details on crude unloading operations and product distributions. They demonstrated that a dynamic model of an integrated supply chain can serve as a valuable quantitative tool that aids in such decision-making. Alabi and Castro (2009) solved a large scale integrated refinery planning using Dantzig-Wolfe and Block Coordinate-descent Decomposition method. Guyonnet et al. (2009) presented a simple MINLP model for an integrated refinery subsystem. However, in their model they considered nonlinearity in the crude oil mix entering the CDU.

2.3.3.6 Future trend in refinery planning

One of the future trends in refinery planning is to find a path towards an automated intelligent refinery that yields profit at its maximum. Increase in available integrated information systems that will improve the comparison of plan versus actual with adjustments for specific real changes from planned feed (Pelham and Harris, 1996).

The need for detailed components and properties characterization of crude oil in order for the amount of products generated from the processing units to be maximized has led to innovation of new technology processes. In this present times, the models and simulators makes use of rigorous computations to characterize and obtain sets of pseudo components which represents the bulk chemical constituents and properties of the crude oil to be processed (Briesen and Marquardt, 2004), this serves as a basis for the commercial simulation software.

The rate of change in the refinery planning and operations was observed by Katzer et al. (2000) to increase in the next 20 years other than the last 70 years. It was discovered that future refinery planning will undertake the molecular characterization of the crude oil before refining. This information will create an increase in the modelling details for adequate processing condition that will reduce sulphur concentration and other environmental emissions to acceptable threshold at low cost (Briesen and Marquardt, 2004).

2.4 Scheduling in oil refineries

Refinery scheduling has attracted an increasing amount of attention in the past decade. The reasons for this are (1) to improve productivity and reduce costs (2) substantial advances of related modelling and solution techniques, as well as the rapidly growing computational power.

Scheduling operations in refinery operations are complex. This has led to developments of optimization models and solution for sub-systems. The following are the three main functional subsystems in a refinery scheduling operations:

- The crude unloading subsystem scheduling
- The production units scheduling
- Products distribution scheduling

The crude oil unloading, storage, blending and charging of CDU is the most essential part of the entire system and it affects the other two subsystems.

2.4.1 Types of Scheduling models

Scheduling of crude oil operations involves two major approaches. They are discrete-time formulation and continuous-time formulation. There also exists a third approach but this is not very popular, it is called the mixed time formulation. In the mixed time formulation, the discrete-time and continuous-time is mixed together.

2.4.1.1 Discrete- time formulation

In discrete time formulation, the scheduling horizon is split into number of intervals of pre-defined duration. However, the duration may not always be equal. All activities such as start and end of the task are compelled to happen within the set boundary of the time horizon. Binary variables are used to enforce a decision as to when a task is carried out within the set boundary. This enables the model to be solved easily. When the problems in the model increase, this increases the size of the binary variables and thereby making the model complex. Problems are usually intractable or require uneconomical computational time and effort when they are large and are represented using discrete time formulation. The accuracy of models depends on size of time interval because discrete- time representation are mere approximation of the real problem. The finer the time interval, the better the results at the expense of computational time and effort, while the larger the time interval, the more the results are suboptimal that are operationally infeasible due to oversimplification of the problem. Bassett et al (1996) described the complexity of scheduling problem that depends on the length of the scheduling time interval, the number of units/equipment involved and the number of tasks and resources available using complex cube.

2.4.1.2 Continuous-time formulation

Continuous- time representation activity start and end time are included explicitly as optimization variables. Continuous time models allows event to take up any time along the scheduling horizon which leads to smaller sizes mathematical models with lesser effort and computational time. This type of representation can be classed into global and unit-specific event based model (Al-Qatahni and Elkamel, 2010).

The optimization algorithm determines the size of the interval. In global event based model, a uniform grid applies to the entire event. While in unit specific event based model, a non-uniform grid where each unit has its own set of time intervals is employed such that task corresponding to the same event point in different units occurs in different times. Most works presented in the literature are global event based (Al-Qatahni and Elkamel, 2010).

Jia and Marianthi (2003) developed a MILP model for gasoline Blending and Distribution Scheduling based on continuous representation of the time domain. They assumed constant recipes for the blending stage. GAMS/CPLEX was used for the solution of the resulting MILP formulation. Again Jia and Marianthi (2004) also developed a comprehensive mathematical model for efficient short –term scheduling of oil refinery operations based on a continuous time formulation.

Moro and pinto (2004) developed a scheduling model for oil refinery operations based on unit specific event point formulation using the state task network representation that was introduced by Kondili et al. (1993).

Comparing the two approaches used for scheduling, continuous time models which allows event to take up any time along the scheduling horizon while in discrete-time formulation the scheduling horizon is split into number of intervals of pre-defined duration which may not always be equal. However, discrete-time based formulation is still popularly used for solving industrial problems (Maravelias and Grossmann, 2006).

2.4.2 Modelling for refinery scheduling

Knowing and including what is relevant and neglecting the issues that are irrelevant for the specific decisions is the key issue that lies in building models of refinery scheduling.

MILP has been widely used for scheduling problems because it is rigorous and flexible, and it has extensive modelling capacity. The application of MILP based scheduling methods ranges from the simplest single- stage single-unit multiproduct processes to the most general multipurpose processes. These process scheduling problems are inherently combinatorial in nature because of the many discrete decisions involved, such as equipment assignment and task allocation over time (Floudas and Lin, 2005).

For large MILP models, the most widely applied technique employed to solve the computational problems is decomposition method (Floudas and Lin, 2005). In this approach, large and computational complex problems are broken down into smaller and easier sub problems which are then solved to global optimality. The solution to the main or parent problem is obtained by integrating optimal schedule of the individual sub problems. Decomposition strategies are classified into time-based decomposition and spatial-decomposition. Researchers have applied the method to decompose large scale MILP scheduling problems. Harjunkoski and Grossmann (2001) applied spatial-decomposition technique for scheduling large steel production model. Basset et al. (1996) adopted the combination of the two strategies based on process recipe. Shah et al. (2009) presented a general novel decomposition scheme which spatially breaks down the refinery scheduling problem into sub problems, which when solve to optimality are then integrated to obtain optimal solution for the whole problem.

They decomposed the whole refinery operations into three categories namely, crude oil unloading and blending, production unit operations and product blending and delivery. There are commercially available software for scheduling operations in the refineries, some are as follows:

- Process Industries Modelling Systems (PIMS) from AspenTech,
- Ominisuite and PetroPlan: These two are for short term scheduling (Li, 2004).

Commercial tools for production scheduling are few and these do not allow a rigorous representation of plant particularities. For this reason, refiners are developing in house tools strongly based on simulation (Pinto et al., 2000).

2.4.3 Recent advances in refinery scheduling

2.4.3.1 Crude oil unloading subsystem scheduling

Supply of crude to the refinery takes place at the crude oil unloading area, which consists of vessels, storage tanks, charging tanks and docking station.

In the crude oil unloading subsystem of the refinery, models have been developed, this include that of Lee et al.(1996) who addressed the issue of inventory management of a refinery that imports several types of crude oil which are delivered by different vessel with MILP. In their paper they reported a short-term scheduling of crude oil inventory management issue that has to do with crude oil unloading from vessel to storage and from storage to charging tanks and finally to the CDU. They linearized the bilinear formulation for the mixing equation by replacing it by individual component flow. They have also assumed sulphur to be the only specific key component in their blended or mixed crude before being fed to the CDU. This is due to the fact that viscosity and other properties of mixed crude are hard to obtain.

Shah (1996) reported an MILP model for crude oil scheduling. In his formulation, the problem was decomposed into an upstream sub problem considering off loading and storage in portside tanks, and a downstream sub problem involving charging tanks and CDU operation. The objective of the work was to minimise tank heels. Sulphur content was also considered as the major key component of the crude.

Wu et al. (2006) included that a short-term scheduling operation in oil refinery should be viewed from control theory and hence, should be solved by combining enumeration and heuristic instead of using mathematical programming formulation.

Magalhaes (2004) and Pinto et al. (2002) focused on crude scheduling using MINLP. Magalhaes (2004) used both continuous and discrete time formulation. In their work, they developed and integrated model for refinery wide scheduling for current operational practise to be improved.

Li et al. (2002) proposed a solution algorithm and effective mathematical formulation for short-term scheduling of crude oil unloading, storage and processing with different types of oil. They acknowledged the non-convex bilinear constraints generated when calculating crude oil mixing and proposed a solution algorithm that iteratively solves two MILP models and a MINLP. However, their algorithm entails solving the NLP at each iteration.

Reddy et al. (2004) also developed an approach to crude oil scheduling introducing facility such as single-buoy mooring (SBM). They presented a MINLP formulation and a MILP–based solution approach. The motivation behind this was due to the nonlinear nature of crude mix. They concluded that the constraint on the bilinear term of the blending and accumulation of crudes in the storage tank is still missing. If there is a mass accumulation in a unit like the charging tank, using individual component flow and solving the model with MILP in some situation provides inconsistent result.

2.4.3.2 Production unit scheduling

In order to satisfy the demand of the customers, the decision on which mode of operation to be used in each processing unit while minimizing the production cost and considering intermediate storage capacities is carried out by the schedulers in the production units. Magalhaes (2004) reported that Moro (2000) in his PhD work studied some issues related to refinery operations. In his work he initially considers a planning problem to develop a general formulation for this type of problems, time is dealt with aggregately. The formulation developed is a general framework for modelling the refinery process units and tanks and the interrelation among them. The developed formulation was applied to two different refineries planning problems and were solved using NLP. The formulation was then used as a basis to develop a general formulation for scheduling problems, where time is a very important variable and solved as an MILP model. The model was then applied to an LPG system.

2.4.3.3 Product distribution subsystem scheduling

In product distribution area of the refinery, Rejowski and Pinto (2003) presented a model on the product distribution part of the petroleum refinery, a multi-product pipeline and several depots connected to local consumers. Simple transport network between the refinery has been developed, while some focused on the combined blending and shipping, some focused more on blending (Guyonnet et al., 2009).

Pitty et al. (2008) presented a dynamic model of refinery supply chain operation, they considered suppliers and customers, functional departments in the refinery, production units and refinery economics. However, their model did not provide explicit details on crude unloading operations and product distributions. They demonstrated that a dynamic model of an integrated supply chain can serve as a valuable quantitative tool that aids in such decision-making.

Alabi and Castro (2009) solved a large scale integrated refinery planning using Dantzig-Wolfe and Block Coordinate-descent Decomposition method.

2.5 Integration of planning and scheduling

The integration of planning and scheduling has received increasing attention in recent years. This is due to refinery interest in improving the overall competitiveness in the global market place by reducing costs and inventories while meeting due dates. While there has been progress towards integrating planning and scheduling, performing simultaneously these tasks still remains elusive. This is due to the fact that simultaneous planning and scheduling involves in principle solving the scheduling problem for the entire planning horizon. This, however, results in a very large scale optimization problem since the problem is defined over long time horizons (Muge and Grossmann, 2007). Dan and Marianthi (2007) indicated that the boundaries between planning and scheduling problems are not well established and there is an intrinsic integration between these decision making stages, lots of work in the literature are addressing the simultaneous consideration of planning and scheduling decisions.

Maravelias and Sung (2009) wrote in their review that planning and scheduling can be integrated following the hierarchical approach where the planning problem is solved first to determine production set target while the scheduling problem is solved to meet these set targets. However, if the scheduling model is used to meet the production target then it will be solved iteratively. If the interdependences of these two levels are not considered at the planning stage, the resulting schedules generated by the schedulers to meet the planning target will be infeasible.

Numerous trade-offs exist between decisions made at the various level of the different subsystems, due to interconnections between the different levels. Therefore, to attain global optimal solutions these interdependences between the different planning functions should be taken into account and planning decisions made concurrently. That is, planning problems should be integrated (Maravelias and Sung, 2009).One model cannot be used for both planning and scheduling, if used will give insufficient information for both levels (Hartmann, 1997).

2.6 Summary

In this chapter, a detailed survey on optimization techniques has been carried out and the disadvantages and advantages of applying LP method were also discussed. Planning in oil refineries and current practice in modelling process units for planning in oil refinery has been extensively reviewed. The review also covered scheduling, its models for the refinery, and current advances in refinery scheduling. Finally, the integration of planning and scheduling were reviewed. From the review, it can be summarised that:

- Despite the disadvantages in using linear models for refinery planning, the advantages supersede. These advantages make LP tools the choice for refinery planning since it is the trend used for most of the simulation packages (Pinto et al 2000). These tools are well developed (Pelham and Harris, 1996). Finally, the required details of refinery processes are captured by linear model formulation (Zhang and Zhu, 2006).

- Rigorous modelling is best applied to process units for planning purposes because of its level of accuracy (Li, 2004).
- An integrated modeling approach in refinery subsystems planning would provide a better link. Also inventory management will be achieved while resolving the issues between the crude oil supply chains (Guyonnet et al., 2009).
- In refinery planning, generally only one crude oil is considered. There is no report of using two or more crude oils in refinery planning. Therefore, it is a knowledge gap to deal with refinery planning with two different crude oils pre-mixed.

In this work, LP shall be the optimization tool to be used. For the process units in the production and product blending subsystem, rigorous modelling shall be used for modelling and finally the planning model derived shall then be used in an integrated refinery subsystem modelling.

3 Rigorous Modelling for CDU and VDU

3.1 Introduction

This chapter focuses on developing and analysing models for CDU and VDU. The CDU and VDU were modelled rigorously in Aspen HYSYS. The flow diagram in Figure 3-1 illustrates the methodological sequence for developing and analysing the CDU and VDU model in this chapter. The CDU model was validated by using data from literature and the summary given in the end.

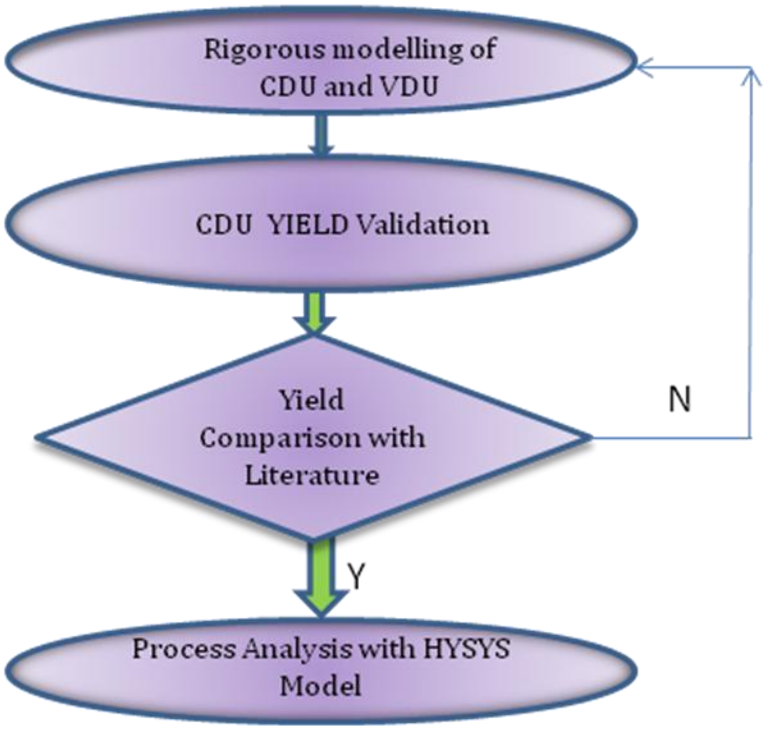

Figure 3-1 Overview of Chapter Methodology

3.2 Process description for the refinery production

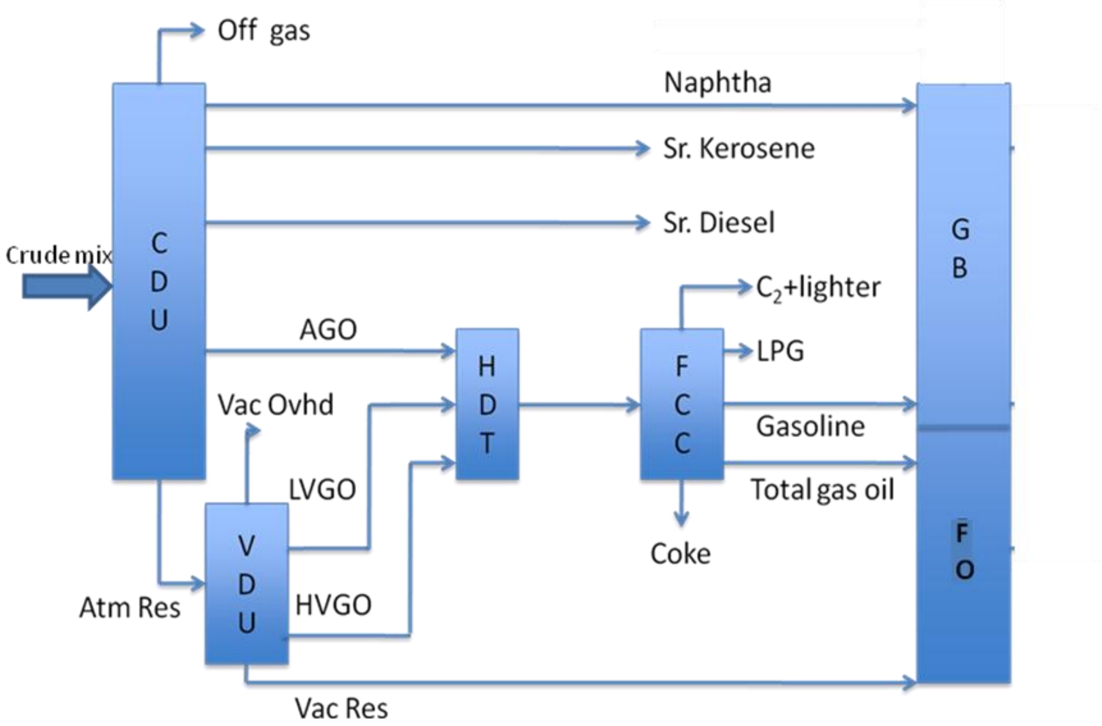

Figure 3-2 Configuration of a Refinery (Arofonosky et al., 1978)

Figure 3-2 is a process flow diagram (PFD) used to describe the process being proposed. The process is made up of five main units namely, CDU, VDU, FCC unit, HDT unit and products blending header. The crude mix or blended crude oil which is comprised of different crudes mixed at a defined volumetric ratios enters the CDU, six different products fraction are obtained which include: Off Gas (OG), Naphtha (N), Straight run Kerosene(Sr K), straight run Diesel, Atmospheric Gas oil (AGO) and Atmospheric Residue (AR). The AR enters the vacuum tower as feed and produces Vacuum Overhead (VO), Low vacuum gas oil (LVGO), High Vacuum Gas oil (HVGO) and Vacuum residue (Vac Res). Naphtha from the CDU and the gasoline from the FCC are further sent to the gasoline blending (GB) header. The LVGO and HVGO from the vacuum tower and the AGO from the atmospheric tower are sent to the HDT for sulphur removal before entering the FCC for further processing and the following intermediates are produced: C2 + lighter, Liquefied petroleum gas (LPG), gasoline, coke and total gas oil (TGO). Vacuum residue from the vacuum tower and the TGO from the FCC are sent to the Fuel-oil (FO) blending header for No. 6 Fuel oil production (Arofonosky et al., 1978).

3.3 Modelling of CDU and VDU in Aspen HYSYS®

In Aspen HYSYS® the modelling of the CDU and VDU was carried out in the following sequence:

- Crude oil characterisation
- Blending of the crudes in different volumetric ratios
- Modelling of pre-Heating train
- CDU modelling
- VDU modelling
- Validation of CDU model

Aspen HYSYS is a modular mode simulation tool. Process equations which relate the outlet stream and the performance variables of a unit to the inlet stream variables are grouped within unit operation blocks. Each unit operation block is then solved one at a time in a sequence with the output of one block becoming the input to another. The direction of flow of information usually follows the material flow (Aspen HYSYS, V7.2).

3.3.1 Crude oil characterization

In crude oil characterization, the feedstock for the CDU which is made up of two types of crude oil were blended to form one crude mix before being processed into different products as demanded. Crude characterisation is usually the first step taken to facilitates other calculations and the minimum requirement are: (a) *whole crude True Boiling Point (TBP) curve,* (b) *whole crude American Petroleum Institute (API) gravity and* (c) *whole crude light ends analysis* (Watkins 1979). Crude is characterised to provide a good representation of it during modelling. A good start is acquiring a distribution curve of a crude assay such as the TBP. Other useful data include property curves like density and viscosity as well as bulk properties. Aspen HYSYS was used to carry out a rigorous steady state modelling with the supplied assay data of the two different crudes to generate internal TBP, sulphur and viscosity curves of the crude mix. The properties and types of the crude used for the oil characterisation are in Table 3-1 and Table 3-2 while the assay of the crudes used can be found in Appendix A.

Table 3-1 Crude oil types and properties

Properties	Ratawi	Brent
API	24.5	38.5
Sulphur wt. %	3.88	0.43
Viscosity (cp)	118.8	4.98
Molecular weight	320	209

Table 3-2 Sulphur concentration, API and Viscosity in the crude oil mixture

Volumetric mixing ratio	Sulphur (wt. %)	API	Viscosity (cp)
0/100	0.43	38.50	4.98
2/98	0.46	34.96	4.07
4/96	0.50	34.81	4.15
25/75	1.02	33.45	5.59
40/60	1.79	29.85	15.78
50/50	2.11	30.98	23.48
60/40	2.47	27.36	32.26
75/25	2.97	25.54	54.92
100/0	3.88	24.50	118.80

From the crude assay data, the distillate production and product distribution from the crude mix was then estimated. In Aspen HYSYS the minimum amount of information required for crude characterization are distillation curve and at least one of the following bulk properties: molecular weight, Density, or Watson K factor.

The light ends of the whole crude that is the pure components with low boiling points was not provided for the crude used, so Aspen HYSYS was used to automatically calculate the light ends of the blended crude by interpolation. These are components in the boiling range of C2 to n-C5.

3.3.2 Blending or mixing of crude oil

Petroleum mixtures used as feedstock in the atmospheric tower are made up of several hundreds of components. Modelling all these components is really not feasible. Therefore, petroleum fractions are used in modelling. These are represented as pseudo-components, characterised by the average boiling point extending over a range of 5-10^{o} C and the fraction density (Huang, 2000).

Two different types of crude were blended at different volumetric ratio e.g. 50/50. Blends are determined based on the design configuration of the CDU. The blended crude can be characterised as sour crude due to high sulphur content (2.11 wt. %). In the blend, Aspen HYSYS automatically cuts the oil into 43 pseudo-components and blended the two assays into one set of pseudo-components. Table 3-3 lists the properties of the 43 pseudo component.

3.3.3 Pre-Heat train

The heat train is comprised of heat exchangers and furnaces. For simplicity, the detailed modelling of the heaters and furnace shall not be dealt with in this work but would be modelled as a simple heater.

Table 3-3 Pseudo Components and Physical Properties of crude oil mix

Comp..Name	NBP (°F)	Mol. Wt.	Density (API)	Viscosity 1 (cP)	Viscosity 2 (cP)	Watson K
NBP_110	109.6572	82.29238	80.63242	3.22E-10	1.05E-10	12.42523
NBP_137	136.9998	86.38583	75.44255	1.60E-02	5.32E-03	12.31227
NBP_164	163.5259	97.80189	61.03144	1.93E-02	5.97E-03	11.62216
NBP_189	188.8577	102.7134	58.37977	2.03E-02	6.08E-03	11.61534
NBP_213	213.1707	109.449	56.12497	2.01E-02	6.11E-03	11.61908
NBP_241	240.8172	114.833	53.30542	2.70E-02	8.28E-03	11.59912
NBP_267	266.7704	121.5616	51.16321	2.79E-02	8.46E-03	11.60454
NBP_292	291.604	129.0114	49.00944	3.06E-02	8.60E-03	11.59693
NBP_318	318.061	135.1389	46.39778	4.56E-02	1.12E-02	11.56176
NBP_344	344.3656	139.2865	44.89812	5.67E-02	1.37E-02	11.59211
NBP_371	370.6562	148.1015	42.53774	7.82E-02	1.85E-02	11.56032
NBP_397	396.8318	155.8196	41.02245	9.83E-02	2.25E-02	11.57885
NBP_423	422.9229	166.7885	39.2412	0.131533	2.80E-02	11.57449
NBP_449	448.901	178.5111	37.64467	0.192253	3.43E-02	11.57768
NBP_475	474.765	192.1125	35.97294	0.281984	4.03E-02	11.57101
NBP_501	500.6102	205.5723	34.39887	0.440065	5.16E-02	11.56697
NBP_527	526.7237	218.6931	32.93148	0.700064	6.46E-02	11.56765
NBP_553	552.8504	233.3523	31.4009	1.085616	7.81E-02	11.56028
NBP_579	578.8869	249.7987	29.90041	1.491025	9.58E-02	11.55114
NBP_605	604.9589	265.6074	28.64219	1.921181	0.119293	11.55621
NBP_631	631.1607	283.6535	27.29981	2.414852	0.145585	11.55259
NBP_657	657.2655	300.6864	26.00811	3.026131	0.178205	11.5493
NBP_683	683.0257	315.8744	24.86838	3.467623	0.216761	11.55321
NBP_709	708.5046	333.221	23.71413	4.52638	0.272423	11.55254
NBP_735	734.6736	390.9735	22.49214	6.843832	0.709777	11.54654
NBP_761	761.024	471.4655	21.44972	9.389477	2.285399	11.55211
NBP_787	786.8905	547.3737	20.46646	11.63377	5.430985	11.55835
NBP_823	823.4059	618.4999	19.29659	13.56353	10.32791	11.58028
NBP_874	874.0338	721.0835	17.64109	16.85143	44.41249	11.60185
NBP_925	924.5961	864.6155	15.92057	22.07416	239.8425	11.61114
NBP_975	975.2554	1031.628	14.20575	28.03564	1300.467	11.6144
NBP_1025	1025.373	1197.455	12.6485	35.64969	7792.487	11.62251
NBP_1072	1072.085	1366.691	11.14675	46.80521	54790.5	11.62078
NBP_1119	1118.76	1535.381	9.611797	96.11141	503669.1	11.61133
NBP_1170	1169.634	1682.915	8.174267	2351.121	3473069	11.61522
NBP_1267	1267.396	1844.002	6.648318	4486162	47900123	11.71365
NBP_1379	1378.731	2068.365	4.204098	2E+11	2.39E+09	11.74852
NBP_1422	1422.462	2255.771	2.133449	3.01E+15	2.21E+10	11.66027
NBP_1559	1559.338	2302.5	0.283276	1.02E+19	1.27E+11	11.77109
NBP_1625	1625.063	2316.671	-1.34169	1.70E+21	4.76E+11	11.75075

NBP_1690	1689.971	2328.181	-2.54611	4.36E+22	1.13E+12	11.76161
NBP_1763	1763.472	2341.618	-3.89724	2.25E+24	2.76E+12	11.76954
NBP_1888	1887.707	2367.475	-6.4602	8.44E+25	7.09E+12	11.74409

3.3.4 CDU modelling

Aspen HYSYS was used to develop a generic model for the CDU, using a column model, solved using HYSIM –Inside-out method which involves the principle of a single equilibrium stage. Peng-Robinson (PR) equation of state is used as fluid package. PR is used because over the years it has been updated for improved calculation of vapour- liquid equilibrium (VLE) (Aspen HYSYS V7.2). The Soave-Redlich-Kwong (SRK) and PR equations have been tested on hydrocarbon mixtures, with both giving nearly similar results (Sim and Daubert, 1980).

The yield prediction from Aspen-HYSYS for the blended crude in the CDU is shown in Table 3-5. The main specification for each intermediate or yield is the boiling range of its components. The boiling range specification for the hydrocarbon stream is expressed by either ASTM 95% points or the TBP endpoint. The ASTM 95% represents the temperature corresponding to 95% vaporisation on the ASTM D86 distillation curve, while the TBP is the temperature at which the whole fraction vaporises on the TBP curve. The TBP and ASTM D86 curve for the crude mix in this work is shown in Figure 3-3.

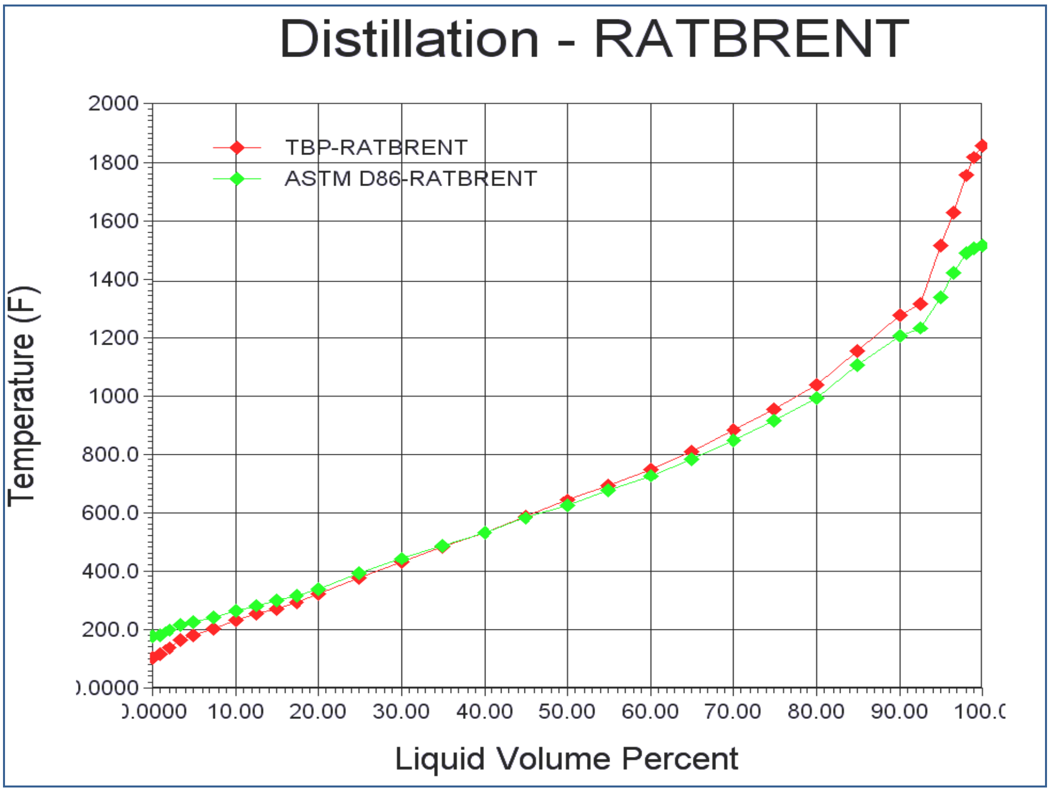

Figure 3-3 TBP and ASTM D86 curve for the crude mix

The fractional distribution of each cut is analysed with the curve when it is plotted against volumetric yield of the cuts. The TBP volumetric yield curve of the individual crude oil entering the CDU was found in the crude assay otherwise it can be provided by the refinery. Table 3-4 shows the volume percent of products distilled at different temperature.

The values of the CDU fractions obtained in Aspen HYSYS are in volume fraction as shown in Table 3-5 but the current practice provides CDU fractions in weight or volume percent. This leaves us with the conversion from volume to weight. For this conversion to be obtained, the $\mathrm{API@60^0F} = \frac{141.5}{\mathrm{Sp.Gr}} - 131.5$ was used. Table 3-6 shows the conversion to volume percent. In all the Tables 3-4, 3-5, and 3-6 below the off gas component of the products from the CDU as shown in the Figure 3-2 was not part of the products listed, this is because of the insignificant quantity of the off gas generated in the CDU with this crude mix. The off gas will subsequently not appear in the list of products yield from the CDU. However, this may vary from crude oil to crude oil.

Table 3-4 TBP and volume percent distilled

Vol. % Distilled	Temp. (oF)	Sulphur Content (Wt. %)
10	236.51	0.0623
20	322.60	0.2285
30	436.60	0.6278
40	538.82	0.9332
50	646.42	1.0958
60	754.66	1.4837
70	885.78	2.0825
80	1040.63	3.2703
90	1282.84	5.1094
95	1520.49	6.8619
100	1859.34	11.6034

Table 3-5 The mixed crude Fractions TBP (^oF) cut point Specification using Aspen HYSYS prediction

Comp. Name	IBP (^oF)	EBP(^oF)	Vol. Fraction	Mass Fraction
Naphtha	158	356	0.2291	0.195
Kerosene	356	554	0.0978	0.090
Diesel	554	644	0.1708	0.165
AGO	644	698	0.0520	0.052
Atm. Residue	698	1859	0.4503	0.497

IBP, Initial Boiling Point. EBP, End Boiling Point

Table 3-6 The mixed crude cut point Specification at ASTM D86using Aspen HYSYS prediction

Products	ASTM95%(^oF)	Sulphur. (Wt. %)	Flow rate (m3/h)	TBP (oF)	Vol.%	Wt. %
Naphtha	318.7	0.0992	137.70	337.10	20.10	16.85
Kerosene(Light Distillate)	446.5	0.4300	67.64	472.70	9.87	7.70
Diesel(Heavy Distillate)	633.1	0.9008	117.20	676.80	17.10	14.23
AGO	733.9	1.2130	35.33	774.60	5.15	4.37
Atm. Residue	1534	3.5300	327.80	1712	47.80	56.90

3.3.5 VDU modelling

As the reduced crude leaves the CDU, it is re-heated in the vacuum furnace and fed into the vacuum tower with vacuum steam. The primary purpose of the vacuum steam is to reduce the hydrocarbon partial pressure in the flash zone of the vacuum tower. When the hydrocarbon partial pressure in the flash zone is lowered, vaporisation takes place and hence distillate production. The specification for the vacuum gas oil is also in form of TBP. The approach used for the CDU is also used for VDU. The yields at TBP and yields at ASTM D86 are summarised in Table 3-7 and Table 3-8 respectively as predicted by Aspen HYSYS for the blended crude. Figure 3-4 is the schematic of the generic CDU and VDU model developed in Aspen HYSYS.

Table 3-7 Vacuum Tower Fractions TBP (^{o}F) cut point Specification predicted by Aspen HYSYS

Comp. Name	IBP (oF)	EBP(oF)	Vol. Fraction	Mass Fraction
Vac. Ovhd	110	698	0.5497	0.502
LVGO	698	806	0.0934	0.0963
HVGO	806	1040	0.1564	0.1676
Vac Residue	1040	1859	0.0223	0.2335

IBP, Initial Boiling Point. EBP, End Boiling Point

Table 3-8 Cut point Specification at ASTM D86 for Vacuum Tower predicted by AspenHYSYS

Products	ASTM 95% (^{o}F)	Sulphur (wt %)	Flow rate (m3/h)	TBP (^{O}F)	Wt.%	Vol. %
Vac. Ovhd	432.3	0.046	2.26	456.3	0.67	0.68
LVGO	681.4	1.057	32.33	718.3	8.82	9.76
HVGO	873.5	1.702	90.62	929.1	26.08	27.37
Vac Residue	1612	4.617	205.80	1812.0	64.47	62.17

Since proper operation of the CDU, VDU, FCC, and HDT with regard to side products cut points leads to meeting the economic objective of a refinery, this work is focused on only these four units. For simplification, the other auxiliaries like the pre-heat train, the desalter and the separator as shown in Figure 3-4, were not modelled in detail.

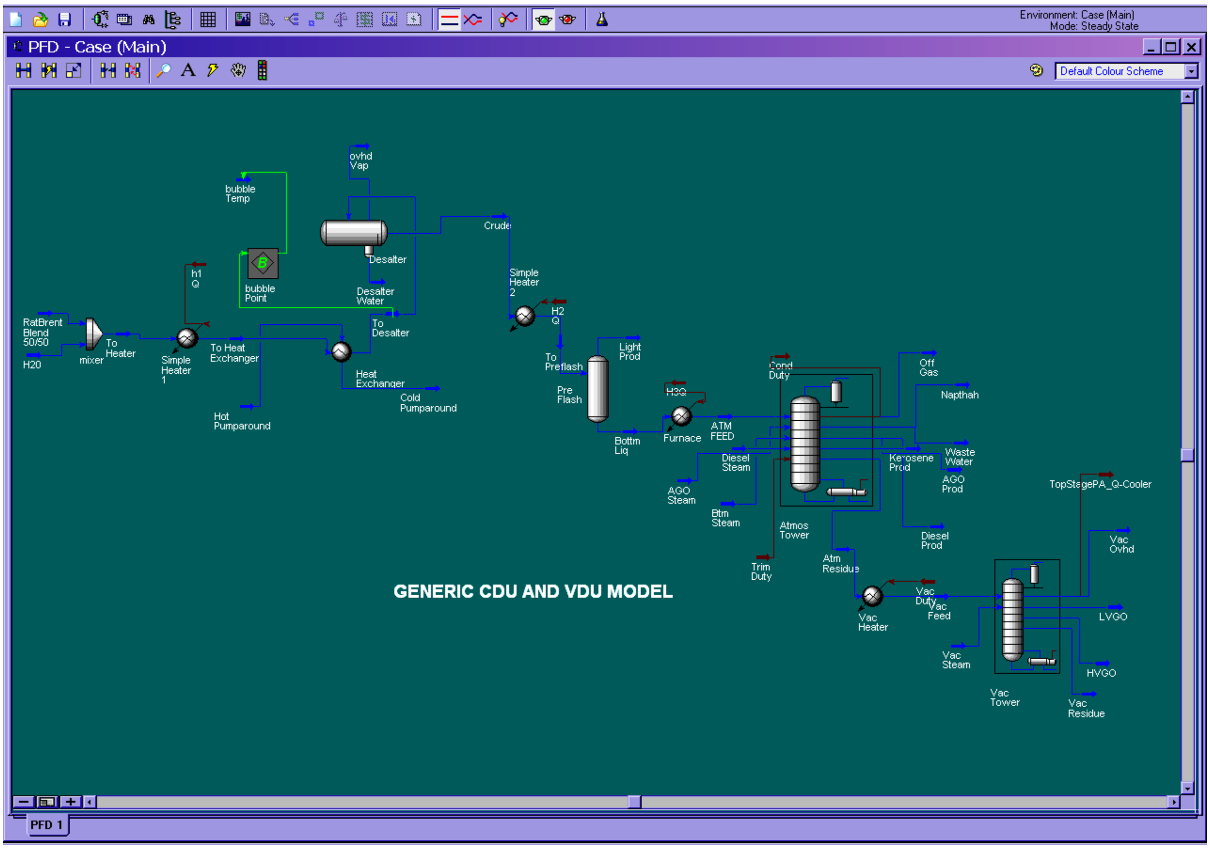

Figure 3-4 Generic CDU and VDU model in Aspen HYSYS

3.3.6 *Validation of CDU model*

The product yields from CDU model in Aspen HYSYS were validated to show that the yields can match with what is in the literature. A Venezuelan crude oil was taken from Li et al. (2005) which is the same as in many other literatures like Alattas et al. (2011), Watkins (1979) and simulated based on the TBP cut points obtained from the crude assay at a throughput of 100,000 barrel per day (BPD). The bulk properties of the crude oil is listed in Table 3-9 while its cut fraction ranges from the distillation unit is shown in Table 3-10.

Table 3-9 Bulk properties of Tia Juana crude oil (Venezuela), (Watkins, 1979)

Vol. % distilled	T(°F)
0	205.99
5	242.01
10	216.28
30	460.73
50	643.62
70	859.20
90	1076.60
95	1127.10
100	1174.70
Bulk Properties	
API	31.6
SG	0.8686
Sulphur (wt %)	1.08
Viscosity: (cp)	
Kinematic cst, @ 70°F	16.1
Kinematic cst, @ 100 °F	10.2

Table 3-10 TBP ranges of CDU fractions (Li et al., 2005)

CDU Fractions		Boiling Range (^oF)
GO(Gross Overhead)	EBP	276.5-290.9
HN (High Naphtha)	IBP	234.4
	EBP	340.6-418.4
LD (Light Distillate)	IBP	257.3-325.1
	EBP	577.9-631.1
HD(Heavy Distillate)	IBP	488.6-545.0
	EBP	711.3
BR(Bottom Residue)	IBP	611.8-630.6

The crude oil cut fractions or yields were estimated in CDU model in Aspen HYSYS and the yield generated were compared with those obtained from literature. The relative percentage errors were calculated. The validation for the Aspen HYSYS model was carried out under the same conditions of EBP temperature of the maximizing heavy naphtha mode (MN) as the main case of Li et al. (2005) and Alattas et al. (2011). Gross overhead was also included for validation because it is included in the data provided by Li et al. (2005). Li et al. (2005) made use of empirical correlations but in this work, rigorous model is used and the results obtained. However, the rigorous model needed to be compared with other method. The CDU fractions obtained matched with Li et al. (2005). The result obtained is shown in Table 3-11 and a chart is also plotted for better view of Aspen HYSYS validation results as seen in Figure 3-5.

Table 3-11 Comparison of product yields from CDU model in Aspen HYSYS and Li et al. (2005)

Products	Empirical-(Li et al. 2005)(Vol. %)	Rigorous-(This work) (Vol. %)	Relative Error (%)
GO	13.61	13.69	0.5
HN	10.60	11.73	9.6
LD	20.98	21.10	0.5
HD	6.91	6.97	0.9
BR	47.04	46.50	1.1

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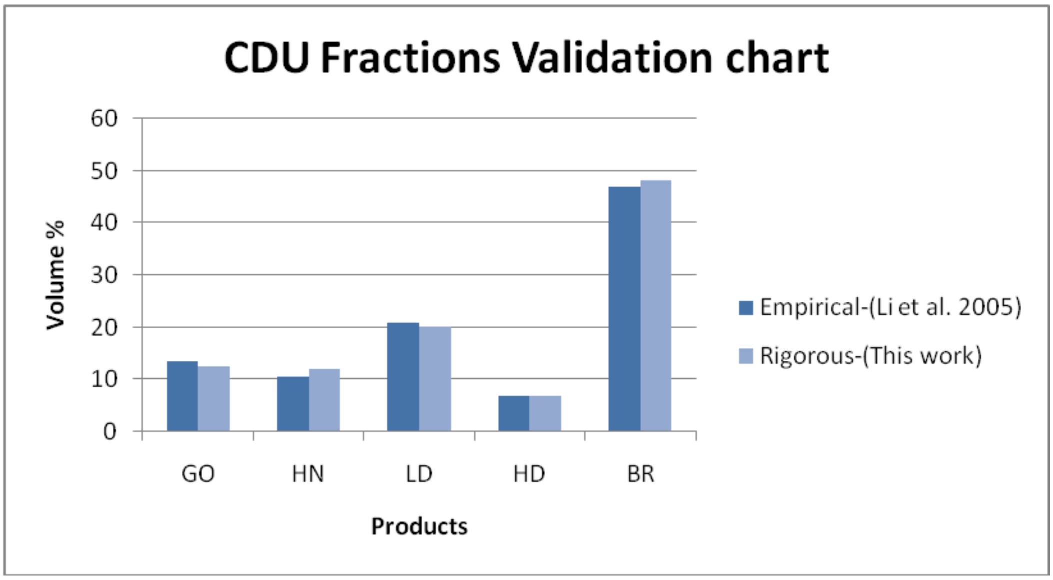

Figure 3-5 Comparison of product yields from CDU model in Aspen HYSYS and Li et al. (2005)

From Table 3-11 and Figure 3-5conclusion can be drawn that the CDU fractions obtained from Aspen HYSYS is a true representation of the product cuts.

The cut fractions or yields from Aspen HYSYS model were also validated using the ASTM D86 TBP from Aspen HYSYS and correlation from literature e.g. Li (2000) polynomial regression method.

Table 3-12 shows the comparison between ASTM D86 to TBP. The ASTM D86 values were obtained from the Aspen HYSYS model. The table does not contain products yields like gross overhead from the CDU because the polynomial regression method used for the comparison in Li (2000) does not contain it either. The names of the products yields as listed in Table 3-12 is the same as used in Li (2000). This has been maintained for proper validation of the CDU.

Table 3-12 Conversion of ASTM D86 to TBP

S/N	Products Names	ASTM D86 (^{O}F)	TBP (^{O}F)	
			(Li 2000) Regression	Aspen HYSYS
1	Naphtha	318.7	335.7	337.1
2	Kerosene	446.5	467.9	472.7
3	Diesel	633.1	664.7	676.8
4	AGO	733.9	773.9	774.6
5	Atm- Res	1534.0	1573.3	1712.0

The plot of the conversion approach was matched with Aspen HYSYS values as shown in Figure 3-6.

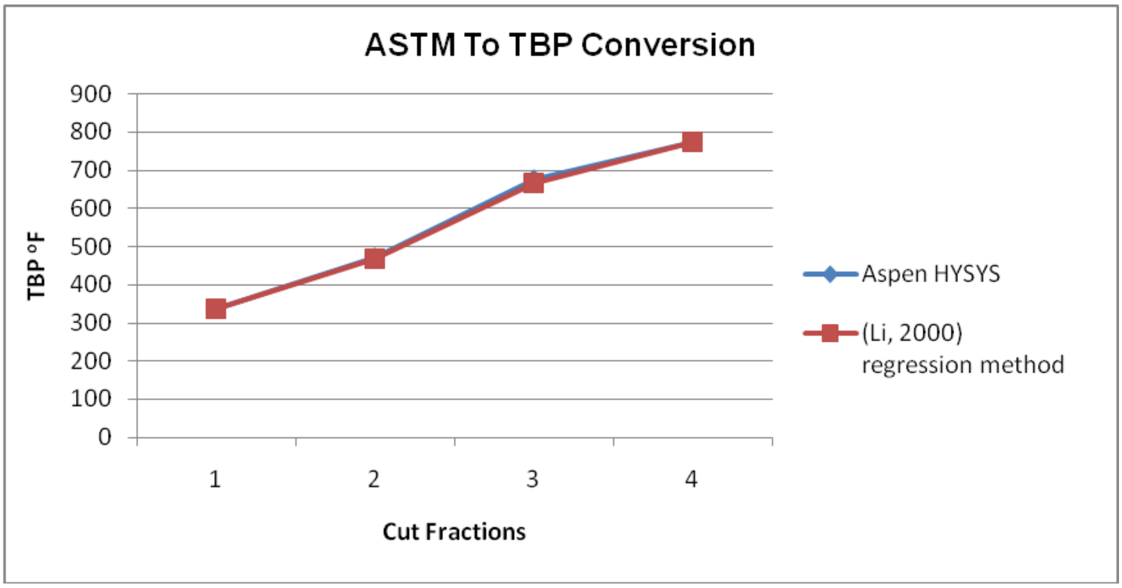

Figure 3-6 Conversion of ASTM to TBP (using Li, 2000)

3.4 Process analysis for CDU and VDU under different crude mix ratios

3.4.1 25/75 volumetric mixing ratio

The 25/75 crude mix was also used in Aspen HYSYS for CDU and VDU simulation and the following results on the products yield were obtained and tabulated in Table 3-13.From Table 3-13 for example, the off gas products were not included in the analysis and the previous products from the CDU, this is because during the simulation, the quantity of off gas generated was very small and is considered negligible in the CDU as previously explained. However, in the VDU overhead gas called vacuum overhead is considered due to the quantity generated.

Table 3-13 Product yields from CDU and VDU in HYSYS for 25/75 mix

Volumetric Blend	25/75		
Products yield	Vol. (m^3/h)	Vol. %	Wt. %
Naphtha	180.8	25.77	22.50
Kerosene	75.11	10.71	9.98
Diesel	127.1	18.12	17.82
AGO	37.89	5.39	5.55
Atm- Res	281.7	40.09	44.14
Total		100	100
Vac Ovhd	2.68	0.95	0.93
LVGO	26.21	9.24	8.42
HVGO	41.93	14.38	14.07
Vac res	212.80	75.54	76.59
Total		100	100

3.4.2 75/25 volumetric mixing ratio

The 75/25 crude mix was also used in HYSYS for CDU and VDU simulation and the following results were obtained and tabulated in Table 3-14.

Table 3-14 Product yield from CDU and VDU from HYSYS for 75/25 crude mix

Products yield	Vol. (m^3/h)	Vol. %	Wt. %
Naphtha	132.90	19.71	16.47
Kerosene	60.34	8.95	8.10
Diesel	108.60	16.11	15.47
AGO	33.34	4.94	4.93
Atm. Res	339.10	50.29	55.04
Total		100	100
Vac- Ovhd	2.71	0.79	0.74
LVGO	32.38	9.44	8.54
HVGO	54.62	15.92	15.01
Vac res	253.4	74.68	75.70
Total		100	100

3.4.3 50/50 volumetric mixing ratio

The 50/50 crude mix was used in Aspen HYSYS for CDU and VDU simulation and the following results were obtained and tabulated in Table 3-15.

Table 3-15 Products yield from CDU and VDU in HYSYS for 50/50 mix

Products yield	Vol. (m^3/h)	Vol. %	Wt. %
Naphtha	156.60	22.84	19.52
Kerosene	67.65	9.87	9.12
Diesel	117.10	17.08	16.64
AGO	35.70	5.21	5.30
Atm Res	308.60	45.01	49.42
Total		100	100
Vac Ovhd	2.26	0.75	0.71
LVGO	29.29	9.40	8.50
HVGO	48.43	15.04	14.68
Vac res	231.50	74.82	76.11
Total		100	100

3.4.4 Analysis of the results on the different crude mix proportions

Appendix H is the summary of the quantities of various yields obtained from the different crude mix proportion simulated in Aspen HYSYS for CDU and VDU.

The blend ratio was observed to affect the yield quantity. Ratawi crude is heavy and sour while Brent crude is sweet. From Appendix H, it was noticed that as the volume ratio of Ratawi crude increases, the quantity of heavy products yields like AGO, Atm. Res, Vac Res and TGO increases. Likewise, if the volumetric ratio of Brent increases, there will be more of the lighter products yields like naphtha, kerosene and fuel gases. This variation is largely due to changes in the crude mix density in the different proportions. The property of crude mix like sulphur, density and viscosity affects the final product yields of interest. If the refiner wants more of heavy products, he will consider the API density of the crude. While the sulphur content of the crude determines the refining requirement to meet the quality specification of the final product yields. The sulphur in the crude mix also affects the cost of the crude and this relatively affects the profit of the final products. From Appendix H conclusion can be drawn that the values obtained from Aspen HYSYS are good representation of industrial and experimental data.

From the two crudes selected (Ratawi and Brent), the more Ratawi crude in the crude mix ratio, the more the refining requirement due to its high sulphur content.

3.5 Summary

In this chapter, the following were carried out

- A rigorous CDU and VDU model was developed using Aspen HYSYS® with two crude oils mixed together in different volumetric mixing ratios.
- The CDU model from Aspen HYSYS® was validated and the results obtained showed that the products cuts from the rigorous model developed are a good representation of CDU cut fractions.
- The rigorous model for CDU and VDU were then used to simulate more volumetric ratios. e.g. 0/100, 2/98, 4/96, 8/92, 10/90… 100/0, etc. It was noticed that as the volume ratio of Ratawi crude increases, the quantity of

heavy products yields such as AGO, Atm. Res, Vac Res and TGO increases. When the volumetric ratio of Brent increases, there will be more of the lighter products yields such as naphtha, kerosene and fuel gases.

4 Refinery Production and Product Blending Subsystem Planning Based on Fixed Yield Approach

4.1 Introduction

In this chapter, the information on products yield obtained from the rigorous and empirical modelling on the various units e.g. CDU, VDU, HDT and FCC is used to develop a simplified mathematical programming planning model for refinery planning of the production and products blending subsystem based on fixed yield approach.

The information on the crude assay and crude rate, and the cut points of the product from the TBP, which are known priori and simulated in Aspen HYSYS in chapter 3 of this paper, shall be used.

In fixed yield approach, to predict the intermediate products yields and qualities obtained from the processing of the crude mix in the CDU and VDU, a linearization of the approximated results from the rigorous models is used in the refinery planning model. Tabulated values of yield and quality of intermediate products produced for each mode are used as its linear model of the CDU and VDU (Brooks and Walsem, 1999).

The planning model developed is then used to carry out planning under different volumetric ratios (up to 53). A plot of profit against volumetric ratios is obtained.

4.2 Process description

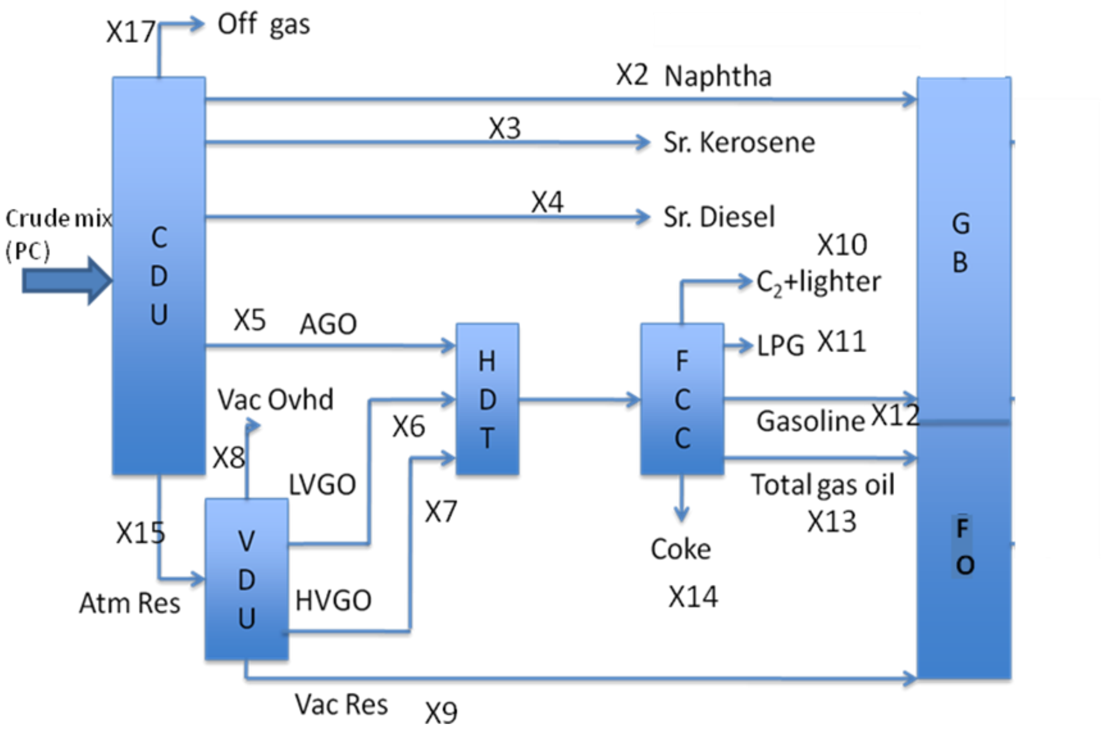

Figure 4-1 Refinery Topology for the Process

Figure 4-1 is a process flow diagram representing a refinery process made up of five main units namely, CDU, VDU, FCC unit, HDT unit and a products blending header. Figure 4-1 is the same with Figure 3-2. However, in this Figure X1-X15 are used to identify the variables for ease of modelling and calculation. The variables, X1-X15 are also used to define the direction of stream flow.

The mixed or blended crude oil enters the CDU; six different product fractions are obtained which includes: Off Gas (OG), Naphtha (N), Straight run Kerosene (Sr Kerosene), straight run Diesel (Sr Diesel), Atmospheric Gas oil (AGO) and Atmospheric Residue (AR). The AR enters the vacuum tower as feed and produces Vacuum Overhead (vac-ovhd), Low vacuum gas oil (LVGO), High Vacuum Gas oil (HVGO) and Vacuum residue (Vac Res). Naphtha from the CDU and the gasoline from the FCC are sent to the gasoline blending header. The LVGO and HVGO from the vacuum tower and the AGO from the atmospheric tower are sent to the HDT for sulphur removal before entering the FCC for further processing and the following intermediates are produced: C_2 + lighter, Liquefied petroleum gas (LPG), FCC-gasoline, coke and total gas oil (TGO). Vacuum residue from the vacuum tower, the TGO from the FCC are sent to the gas oil (FO) blending header for No. 6 Fuel oil production.

4.3 Mathematical programming model for CDU and VDU

The following assumptions were made:

- Perfect mixing is assumed
- There is no accumulation in the units
- The mass balance on yields of individual units is used to determine the product flow rates. These are also function of the feed.
- Bound constraints are satisfied by individual process units.
- The properties of the inlet feed stream is not varying.
- Parameters such as temperature, pressure, heat transfer and energy balance which were used for the process units are not considered in this model.

4.3.1 CDU material balance constraints

The material balance constraints are in the form of inequalities such that output is equal or less than input. This is because equality makes LP models constraining and often prevents finding feasible solutions (Arofonosky et al. , 1978).

Based on fixed yield approach, the material balance for each product stream is obtained by multiplying the feed into the refinery process unit (e.g. CDU) by its coefficient. Therefore, the sum of the entire product coefficients from each unit is equal to unity, on this premix, the following set of equations (Eq. 4-1 to 4-10) is developed for CDU and VDU. For consistency, the feed into any process unit is assigned negative sign indicating it is been consumed in that unit, while product from such unit is positive and all balance constraint are on the right hand side, and equated to zero.

$$X2_{naphtha} - IP_2 \ PC_{cm,t} \leq 0 \qquad (4\text{-}1)$$

$$X3_{kero} - IP_3 \ PC_{cm,t} \leq 0 \qquad (4\text{-}2)$$

$$X4_{diesel} - IP_4 \ PC_{cm,t} \leq 0 \qquad (4\text{-}3)$$

$$X5_{ago} - IP_5 \ PC_{cm,t} \leq 0 \qquad (4\text{-}4)$$

$$X15_{atmres} - IP_{15} \ PC_{cm,t} \leq 0 \qquad (4\text{-}5)$$

$$X17_{offgas} - IP_{17} \ PC_{cm,t} \leq 0 \qquad (4\text{-}6)$$

4.3.2 VDU material balance constraint

$$X8_{ovhd} - IP_8 X15_{atmres} \leq 0 \qquad (4\text{-}7)$$

$$X6_{lvgo} - IP_6 X15_{atmres} \leq 0 \qquad (4\text{-}8)$$

$$X7_{hvgo} - IP_7 X15_{atmres} \leq 0 \qquad (4\text{-}9)$$

$$X9_{vacres} - IP_9 X15_{atmres} \leq 0 \qquad (4\text{-}10)$$

4.3.3 Capacity constraint for CDU and VDU

The feed rates of crude oil to the units, averaged over a period of time can be any value ranging from zero to the maximum plant capacity.

$$PC_{cm} \leq CAP_{cdu,t} \qquad (4\text{-}11)$$

$$X15_{atmres} \leq CAP_{vdu,t} \qquad (4\text{-}12)$$

4.4 Empirical correlations used in mathematical programming model for HDT and FCC units

4.4.1 HDT unit and material balance

Some of the products slates or cuts from the VDU serve as feed to the HDT due to the high sulphur content before being sent to the FCC. The vacuum residue produced from the VDU is sent to the FO header for blending to produce No 6 fuel oil. Since there are very little publications on hydrotreater yields, an empirical method described by Gary and Handwerk (2001) is adopted for this work. 98% of products yield on feed are expected, while other feed conditions remains the same. The yields obtained for 50/50 crude mix are listed in Table 4-1. The method used to calculate the yield for the FCC unit can be found in appendix C. Figure 11.

Table 4-1 Products cuts from Hydro treating of the oils

Products	Yields		Vol. (m^3/h)
	Vol. (%)	Wt. (%)	
LVGO	26.22	24.93	29.29
HVGO	42.47	50.12	48.43
AGO	31.31	24.95	35.70

Implementing the correlation by Gary and Handwerk (2001) on HDT, the material balance constraint is then:

$$X_{16} - 0.98\ [(X5), (X6) \text{and}\ (X7)] \leq 0 \qquad (4\text{-}13)$$

4.4.2 FCC unit and material balance

Feed from the HDT enters the FCC unit. The FCC unit produces cyclic oil, and this oil is blended in the FO header with the vacuum residue from the VDU for the production of No 6 fuel oil. Empirical correlation for FCC by Gary and Handwerk (2001) is adopted in this work. A fixed conversion rate is used.

The properties of the feed from the HDT after reducing the sulphur content by the method proposed by Gary and Handwerk (2001) were obtained. A zeolite catalyst was used and a Watson K factor of 11.8 for the gas oil feed into the FCC. The information on the Watson K factor is obtained from Aspen HYSYS. This is because the feed conditions into the HDT and subsequently into the FCC remained constant from the VDU. The conversion level was obtained with respect to the gas oil feed which is straight run gas oil or straight run plus coker gas oil. In this work the feed is straight run gas oil from the CDU, tracing the K factor to the gas oil curve in Figure 1 in appendix A. 68% conversion level was obtained. The rest of the yields were obtained based on this conversion rate as in Appendix A from Figure 2 to Figure 10.

The values obtained for the FCC product cuts in weight and volume percent for 50/50 crude mix are shown in Table 4-2.

Table 4-2 Yields fraction from FCC

Volumetric Blend	**50/50**		
Products	Vol. (m3/h)	Vol.%	Wt.%
Coke	5.8	3.96	5.20
C_2+liighter	12.11	8.28	5.10
LPG	24.37	16.65	13.72
TGO	44.32	29.53	38.40
Gasoline	59.30	41.56	37.60

$$X10 - 0.0832X_{16} \leq 0 \tag{4-14}$$

$$X11 - 0.1686X_{16} \leq 0 \tag{4-15}$$

$$X12 - 0.4127X_{16} \leq 0 \tag{4-16}$$

$$X13 - 0.2992X_{16} \leq 0 \tag{4-17}$$

$$X14 - 0.0398X_{16} \leq 0 \tag{4-18}$$

4.4.3 Capacity constraint for HDT and FCC units

$$[(X5),(X6)\text{and }(X7)] \leq CAP_{hdt,t} \tag{4-19}$$

$$X16_{hdt} \leq CAP_{fcc,t} \tag{4-20}$$

4.5 CDU and VDU mathematical programming planning model validation

The model developed was validated in GAMS with CPLEX solver. The yields obtained in the 50/50 volumetric ratio in Aspen HYSYS are used to validate the model. This is to determine the efficacy of the model. The CDU capacity of 100,000bbl/day and VDU capacity of 46,500bbl/day were used.

Table 4-3 The Coefficients generated for CDU and VDU in Aspen HYSYS at 50/50 crude mix

Products	Coefficients	Values from Aspen HYSYS Vol. %
Naphtha	IP_2	22.84
Kerosene	IP_3	9.87
Diesel	IP_4	17.08
AGO	IP_5	5.21
ATM RES.	IP_{15}	45.01
LVGO	IP_6	9.40
HVGO	IP_7	15.04
Vacuum Ovhd	IP_8	0.75
Vacuum Residue	IP_9	74.82

Generated products from CDU and VDU in volume percent from GAMS are then compared with the values obtained from Aspen HYSYS and relative difference calculated. The material balance in the individual products streams is obtained by multiplying the feed into the units by its coefficients.

From the validation results in Table 4-4, the relative error ranged from 0.48 to 3.98 which is acceptable range. Table 4-5 and 4-6 shows the split for the different process units.

Table 4-4 Validation results for CDU and VDU

	GAMS		Aspen HYSYS	Relative Difference
PRODUCTS (50/50)	Vol.(kbbl/day)	Vol. (m^3/h)	Vol. (m^3/h)	%
Naphtha	22.84	155.75	156.60	0.50
Kerosene	9.87	67.30	67.65	0.52
Diesel	17.08	116.47	117.10	0.54
AGO	5.21	35.53	35.70	0.48
ATM RES.	45.00	300.04	308.60	2.77
LVGO	4.14	28.22	29.29	3.65
HVGO	6.84	46.66	48.43	3.65
Vacuum Ovhd	0.32	2.17	2.26	3.98
Vac. Residue	32.70	222.98	231.50	3.68

Table 4-5 Validation of CDU model with yield from GAMS

Products	**GAMS**		**Aspen HYSYS**	**Relative Difference**
	Vol. (kbbl/day)	Vol. (m^3/h)	Vol. (m^3/h)	
Naphtha	22.84	155.75	156.60	0.0050
Kerosene	9.87	67.30	67.65	0.0052
Diesel	17.08	116.47	117.10	0.0054
AGO	5.21	35.53	35.70	0.0048
Atm-Res	45.00	300.04	308.60	0.0259
Total	100.00	675.09	685.65	1.54

Table 4-6 Validation of VDU model with yield from GAMS

Products	GAMS		Aspen HYSYS	Relative error
	Vol.(kbbl/day)	Vol. (m^3/h)	Vol. (m^3/h)	
Vac-Ovhd	0.32	2.18	2.26	0.0372
LVGO	4.14	28.22	29.29	0.0365
HVGO	6.84	46.66	48.43	0.0365
Vac-Res	32.70	222.99	231.50	0.0367
Total	44	300.05	311.48	0.0367

It can be observed from the validation Tables 4-5 and 4-6that the CDU and VDU model when implemented in GAMS presented yield with difference ranging from 0.5% to 2.6% for CDU and 3.65% to 3.72% for VDU. Considering the error ranges which are in percentage, the simplified linear Programming models developed are good representation of the CDU and VDU with respect to the cut fractions obtained from Aspen HYSYS. Similarly, Figures 4-2 and 4-3 are plots comparing the volume of product obtained from GAMS and Aspen HYSYS which shows a good match for all the products for the different process units.

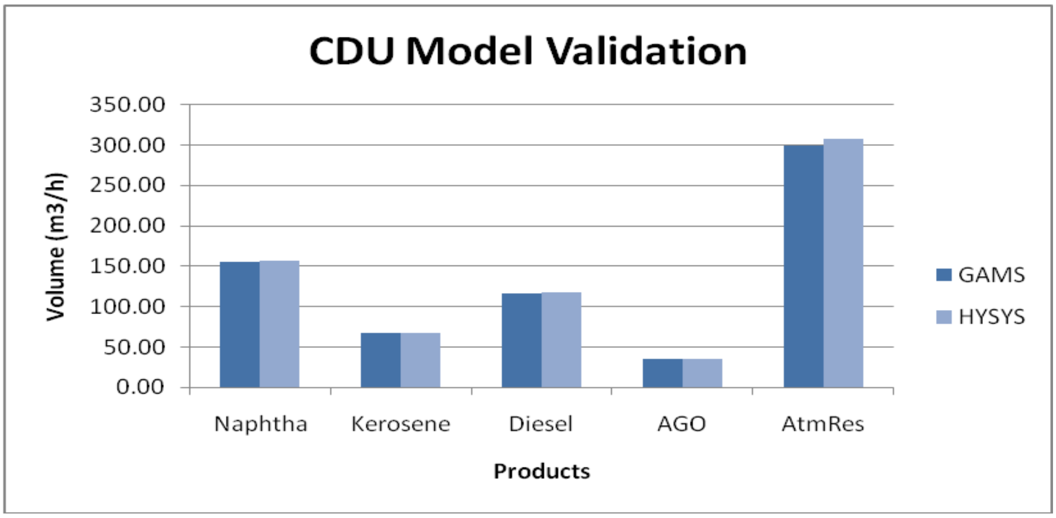

Figure 4-2 CDU yield from Aspen HYSYS model validation with GAMS

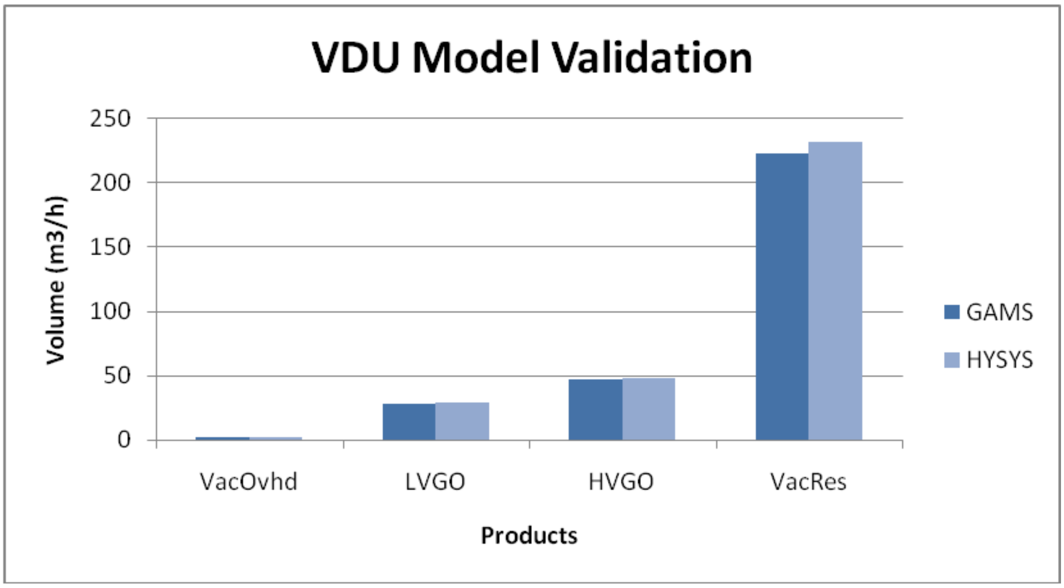

Figure 4-3 CDU yield from Aspen HYSYS model validation with GAMS

Further validation was carried out using the 25/75 volumetric mixing ratios for the CDU and VDU.

Table 4-7 Product yield of 25/75% crude oil mix from HYSYS

Product Yield (25/75 mix)	Vol.(m^3/h)	Vol. %
Naphtha	180.8	25.73
Kerosene	75.11	10.69
Diesel	127.1	18.09
AGO	37.89	5.39
AtmRes	281.7	40.09
Vac ovhd	2.681	0.945
LVGO	26.21	9.245
HVGO	41.93	14.78
Vac res	212.8	75.03

Table 4-8 Validation of yield results for 25/75 volumetric mixing ratio from Aspen HYSYS

Products (25/75)	GAMS		Aspen HYSYS	Absolute error	Relative error %
	Vol. (kbbl/day)	Vol. (m^3/h)	Vol. (m^3/h)		
Naphtha	25.73	175.50	180.80	5.30	2.93
Kerosene	10.69	72.90	75.11	2.21	2.94
Diesel	18.09	123.36	127.10	3.74	2.94
AGO	5.39	36.76	37.89	1.13	2.98
Atm-Res	40.09	273.37	281.70	8.33	2.96
Total	100	681.89	702.6	20.71	2.95
Vac ovhd	0.38	2.58	2.68	0.1	3.72
LVGO	3.71	25.27	26.21	0.94	3.58
HVGO	5.93	40.40	41.93	1.53	3.65
Vac res	30.08	205.12	212.80	7.68	3.61
Total	40.10	273.37	283.62	10.25	3.61

From the validation carried out as tabulated in Tables 4-7 and 4-8 that the CDU and VDU model when implemented in GAMS presented yield with difference ranging from 2.93% to 2.98% for CDU and 3.58% to 3.72% for VDU. Considering the error ranges which are in percentage, the simplified linear Programming models developed are good representation of the CDU and VDU with respect to the cut fractions obtained from Aspen HYSYS.

4.6 Model for refinery production and product blending subsystem planning in GAMS

The planning model in this section for refinery production and products blending subsystem considered two types of balances (Al-Qatahni and Elkamel, 2010); these are

- Fixed plant yield
- Unrestricted balances.

4.6.1 Mathematical model formulation

The material balance for the CDU yield:

Equation (4-19 to 4-22), indicates that the minimum flow into a process unit must be satisfied so as to prevent a no flow condition.

$$IP_{cdu,f,f',cm}PROLEV_{cdu,cm,t} + PC_{cm,t} \geq 0 \qquad (4-19)$$

Material balance for the VDU yield:

$$IP_{vdu,f,f',cm}PROLEV_{vdu,cm,t} + PC_{cm,t} \geq 0 \qquad (4-20)$$

Material balance for the FCC yield:

$$IP_{fcc,f,f',cm}PROLEV_{fcc,cm,t} + PC_{cm,t} \geq 0 \qquad (4-21)$$

The unrestricted balance occurred also in the HDT and therefore, the sum of the gas oils are the feed.

$$PROLEV_{fcc,cm,t} - 0.98 * \sum IP_{fcc,f,f',cm} \geq 0 \qquad (4-22)$$

4.6.2 Capacity constraint

$$\sum_{cm \in CM} PROLEV_{u,cm,t} \leq cap_u \forall_{u,t} \qquad (4-23)$$

4.6.3 Blending Constraint

The intermediates used for blending to produce final products are obtained by the summation of the required or desired constituents, which is represented by the following set of equation.

$$FFP_{fp,t} - \sum_{t} \sum_{fp \in cm} X_{(cm,t)} \geq 0 \qquad (4-24)$$

4.6.4 Market requirement Constraint

Constraints that defines the product requirements over the planning horizon. The maximum production requirement constraint in bbl/day is:

$$FFP_{fp} \leq RM_{fp} \qquad (4-25)$$

4.6.5 Crude oil composition constraint

The sum of the percentage of each crude oil in the crude mix must be equal to 100.

$$\sum_{p=1}^{k} P_{cm} = 100 \qquad (4-26)$$

P_{cm} = crude oil percentage in the crude mix.

4.6.6 Objective function

The objective function is formulated to maximise profit. It is determined as:

Total Revenue generated from final product (REV) minus Total cost of operations (COP)and total cost of crude(IMPCST).

$$\sum_{t\in T} REV_t - \sum_{t\in T} COP_t - \sum_{t\in T} IMPCST_t \qquad (4-27)$$

Total income

This is the total revenue generated from sales of the final products and it is represented in Equation (4-28).

$$\mathrm{REV_t} = \sum \sum_{\mathrm{fp\in FP}} \mathrm{RV_{fp}} \times \mathrm{FFP_{fp}} \qquad \forall \mathrm{t} \qquad (4-28)$$

The cost of crude oil mix and the cost of intermediate materials like butane are the input material cost.

$$\mathrm{IMPCST_t} = \sum_{\mathrm{pmat\in PMAT}} \sum \mathrm{Cost2_{pmat,t}} \times \sum_{\mathrm{cm\in CM}} \sum \mathrm{Cost1_{cm,t}} \times \mathrm{PC_{cm,t}} \qquad (4-29)$$

Cost of operation

The cost of all the refinery units multiply by the level of the process makes up the cost of the refinery operations.

$$\mathrm{COP_t} = \sum_{\mathrm{u\in U}} \left(\mathrm{Cost_u} \times \sum \mathrm{PROLEV_{u,cm,t}}\right) \qquad \forall \mathrm{t} \qquad (4-30)$$

4.6.7 Crude limit constraint

The amount of crude oil that is allowed to feed the CDU,

$$PC_{cm,t} \leq 100 \qquad (4-31)$$

4.7 Refinery planning under different volumetric mixing ratios

53model runs in GAMS is then carried out on 50 different volumetric mixing ratio runs of rigorous models generated from Aspen HYSYS.

The 53GAMS model runs is used to determine the optimal volumetric ratio that generates the highest profit and the sulphur content based on some specified constraint. Other variables like the CDU feed rate and the flow of intermediates were also determined.

4.7.1 Solution strategy

- Up to 53 different volumetric mixing ratios are evaluated in Aspen HYSYS e.g. 0/100, 2/98, 4/96, 6/94, 8/92, 10/90,...., 100/0
- Using the refinery planning model developed in section 4.6,53 mathematical programming planning runs are carried out in GAMS on individual volumetric ratio
- Plot of the profits obtained from the 53 different volumetric mixing ratios versus the individual volumetric ratios is then carried out.

4.7.2 Problem statement and implementation

Two crude vessels are expected to arrive with two different sets of crude: Ratawi and Brent. The refinery has one CDU which has been designed to process a capacity of not more than 100,000 barrel per day as shown in Table 4-9. The refinery is capable of handling any blend of the two crudes at different proportions. It is assumed that the product price and processing cost as shown in Table 4-10and Table 4-11 are the same throughout the 30-day period. The assumption made for the processing cost is due to unavailability of processing cost data at the different volumetric mixing ratio.

In this problem there are eighteen flow rates (i.e. decision or optimization variables), crude input and products output whose optimal values are required in order to obtain the maximum profit. In this case study, the objective is to use the developed model to solve the proposed petroleum refinery problem. The model will be implemented with GAMS using CPLEX solver.

The model since its profit maximization treats the crude oil input and products output as values for the model to determine rather than given.

- Crude flow rate into the CDU
- Quantities of individual intermediates and final products
- Optimal profit
- Which volumetric ratio gave the highest profit

4.7.3 Objective function

A planning horizon of 30 days is used for this case study and each day is a time interval. The objective of the optimisation problem is to achieve maximum profit over the entire planning horizon given the type of crude oil and facilities needed in the refinery to produce various products. The cost of purchasing the crude oil and the cost of processing the crude oil are subtracted from the revenue or income generated from the finished products as stated in equation 4-27.The objective function and all constraints are linear.

4.7.4 Decision variables

The following decision variables have been used in the optimization problem formulation: Flow rates of materials (crude and intermediate) to and from the refinery and the quantities of final products.

4.7.5 Parameters used

Capacity of processing units and the Prices of final products are in Table 4-9 and Table 4-10.

Table 4-9 Capacity of processing units in the Refinery

Processing Unit	Capacity (bbl/day)
CDU	100 000
VDU	46500
FCC	16800
HDT	17140

Table 4-10 Product price for Final Products (EIA 2011)

Final Products	Product price($/bbl)
Gasoline Blend (GB)	**146.25**
Kerosene	**114.12**
Fuel-oil	**111.78**
Fuel-gas	**50.07**
Diesel	**147.24**

Data on operating cost of the units, maximum production limit and product price were obtained from literature as shown in Tables 4-11 and 4-12, while the crude oil mix price is obtained from the volumetric ratios of the crude mix as shown in Table 4-13which are then optimized for 30 days planning horizon.

Table 4-11 Process Units Operating Cost (Ajose, 2010)

Process Units	Operating Cost ($/bbl produced)
CDU	0.59
VDU	0.72
HDT	0.19
FCC	0.41

Table 4-12 Production limit (Ajose, 2010)

Products	Maximum Production Requirement (kbbl)
Gasoline	61.144
Kerosene	20.79
Diesel	36.04
Fuel oil	55.37
Fuel Gas	6.31

Table 4-13 Crude oil and Butane data (EIA 2011)

Crude Oil	cost ($/bbl)
RATAWI	88.58
BRENT	115.93

4.8 Results and analysis

Table 4-14 Summary of the profit generated from different volumetric mixing ratios

scenarios		Profit $/30 Days	scenarios		Profit $/30 Days	scenarios		Profit $/30 Days
0_100	1	28483	36_64	20	59337	72_28	39	77816
2_98	2	35039	38_62	21	60820	74_26	40	78712
4_96	3	36682	40_60	22	61801	76_24	41	79495
6_94	4	37796	42_58	23	63707	78_22	42	80296
8_92	5	39434	44_56	24	64500	80_20	43	80081
10_90	6	40900	46_54	25	66232	82_18	44	80993
12_88	7	42019	48_52	26	67517	84_16	45	81757
14_86	8	43634	50_50	27	70908	86_14	46	81591
16_84	9	44954	52_48	28	70187	88_12	47	82768
18_82	10	46062	54_46	29	71707	90_10	48	83379
20_80	11	47650	56_44	30	72972	92_8	49	83531
22_78	12	48996	58_42	31	73624	94_6	50	83755
24_76	13	50805	60_40	32	75269	96_4	51	83983
25_75	14	50624	62_38	33	74756	98_2	52	84614
26_74	15	51674	64_36	34	75623	100_0	53	84168
28_72	16	52884	65_35	35	75986			
30_70	17	54372	66_34	36	75777			
32_68	18	55556	68_32	37	77022			
34_66	19	57153	70_30	38	76751			

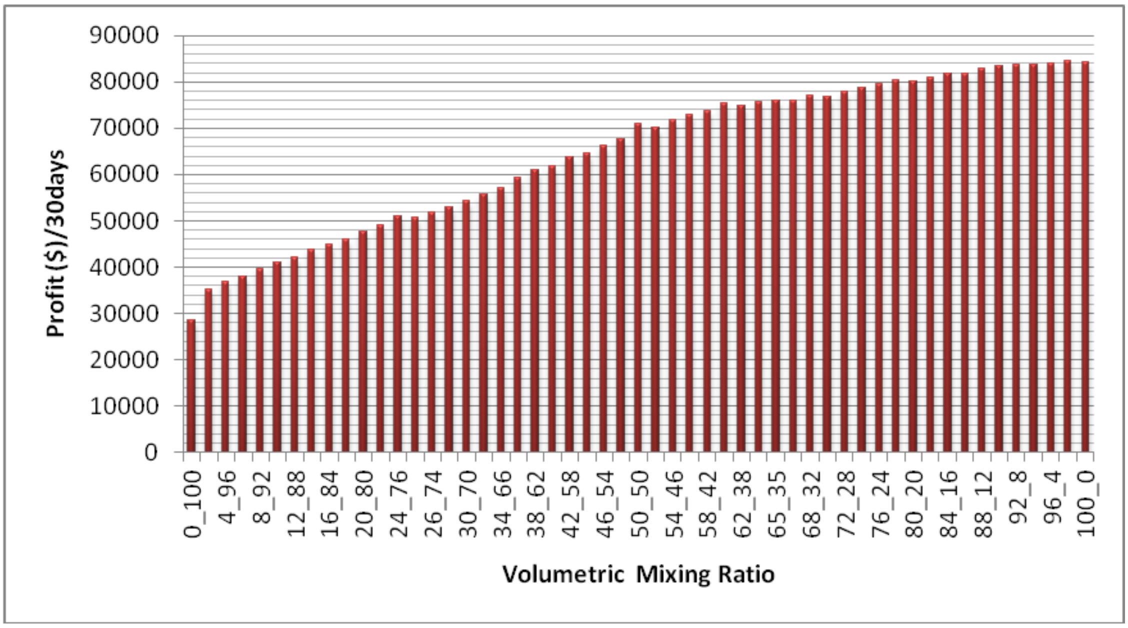

Figure 4-4 Plot of Volumetric ratios versus Profits

Figure 4-4 is a plot of different profit obtained against volumetric ratios or scenarios. From Figure 4-4, when only the Brent crude oil is used, the profit is as low as $28483 for the 30 days planning horizon as shown in Table 4-14. But as soon as the Ratawi crude is introduced into the Brent crude, the profit jumped to $35039, the increase in profit continues not in a straight line but undulating as shown in the same Figure. The plot shows increase in the profit as the volumetric ratio with more sulphur content increases. This is due to the assumption that the operating cost for all the scenarios or volumetric mixing ratios are the same. The cost of the volumetric ratio with more sulphur is less than the cost of the volumetric ratio with lower sulphur content.

In real refinery case data, the cost of processing a more sulphur rich crude may not be the same with the cost of processing a less sulphur rich crude. The variation in processing cost affects the refinery profit. Another aspect of cost that may affect the profit is the blending cost as stated by Robertson et al. (2011). In their paper, they analysed how blending cost that has been ignored by several authors affects profit. The cost for processing has been assumed in this work the same because of lack of real data.

From the results obtained, the highest profit of $84614 was obtained at volumetric ratio of 98% of Ratawi and 2% of Brent crude oil and the sulphur content at this volumetric ratio is 2.655 wt percent. The flow into the CDU is about 84,000bbl/day. The volumetric mixing ratio that gave the highest profit is used as a base case for analysis.

Table 4-15 Summary of results obtained from the refinery planning model using Fixed yield method

Products fractions	Fixed Yield Method (98/2) (Kbbl/day)
Naphtha	14.36
Kerosene	6.96
Diesel	12.99
AGO	4.23
ATM RES.	46.50
LVGO	4.48
HVGO	7.81
Vacuum Ovhd	0.34
Vacuum Residue	34.35
FCC-gas	6.36
TGO	5.01
C2+Lighter	1.35
LPG	2.83
FINAL PRODUCTS (kbbl/day)	
GASOLINE BLEND (GB)	20.72
FUEL-OIL	39.36
KEROSENE	6.96
DIESEL	12.99
FUEL-GAS	4.511
PROFIT ($/30 DAYS)	84614

Table 4-15 is a summary of the results obtained from the volumetric mixing ratio that gave the highest profit. The volume of intermediates and final produced are listed in the table. At the end of the 30 days planning horizon, the profit came out to be $84614 from sale of the final products after every cost has been removed.

Conclusion can be drawn on the use of mixed crude for refinery processing, that the cheaper the crude oil the more the profit.

4.9 Summary

Fixed yield was successfully implemented in planning refinery production and product blending subsystem with the models developed from the information generated from the previous Chapter 3 of this thesis.

- The information from the rigorous and empirical model was used to develop a mathematical programming model for CDU, VDU, HDT and FCC based on fixed yield method.
- The developed model is implemented in GAMS and validated.
- The validated mathematical programming model was then used to implement a case study in a refinery planning model for production and product blending subsystem.
- The proposed two crudes used in chapter 3 of this thesis was mixed in up to 50 different scenarios (volumetric mixing ratios) in Aspen HYSYS model and the volume percent of the different yields obtained. The 53runs of the rigorous model in Aspen HYSYS were then run up to 53 times again in a mathematical programming model for planning in GAMS.
- It was discovered that the highest profit can be achieved in 98/2 volumetric mixing ratio.

From the procedures, the process of obtaining the refinery profit in the various volumetric mixing ratios is cumbersome i.e. the yields for individual products fractions and for individual volumetric ratios are achieved 53 times in Aspen HYSYS and 53 times in GAMS.

5 Refinery Production and Product Blending Subsystem Planning with Aggregate Model

5.1 Introduction

This chapter is aimed at developing an aggregate model for CDU and VDU yield prediction used for refinery planning of the production and product blending subsystem. This is achieved by using the information obtained from the rigorous modelling for the CDU and VDU combined with models (obtained from empirical correlations) for FCC and HDT detailed in chapter3 and 4 solved with CPLEX solver. 53 different volumetric ratios were generated from rigorous model. The generated volumetric ratios were then used to derive regression model with sulphur (x) as the independent variable and the cut fractions or yields (y) as the dependent variables. The derived regression models were then used in place of the regular fixed yield in the refinery production and products blending subsystem planning model. An overview of the procedure is presented in Figure 5-1.

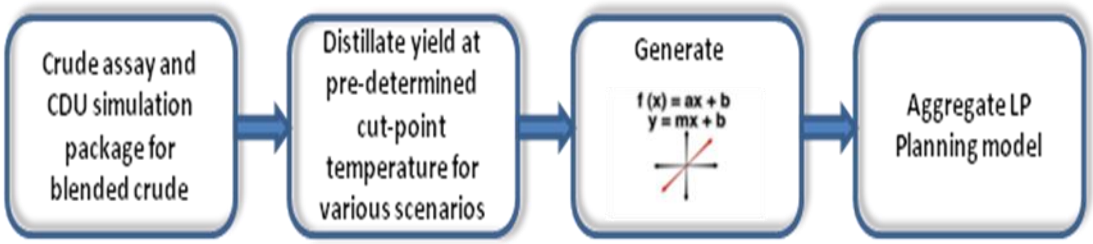

Figure 5-1 Procedures for Developing Aggregate Model

The same case study as in chapter 4 was then used to demonstrate the applicability of the proposed method and solution approach.

5.2 Derivation of regression model for CDU and VDU with information from rigorous model

5.2.1 Determination of factor that is used as independent variable

Linear regression is used in this work to estimate the effect of changing the sulphur content in crude mix (X) which is an independent variable over yields (Y) the dependent variable or to find the line that best predicts Y from X. This idea is inspired by Robertson et al. (2011).

Some of the 53 different volumetric mixing ratios that were generated from rigorous model and the properties at the different volumetric mixing ratio such as sulphur, API and viscosity are shown in Table 5-1. Sulphur is one of the key components of crude oil that determines if a crude oil is expensive (sweet) or not (sour).

Table 5-1 Different volumetric mixing ratios and their properties

Volumetric mixing ratio	Sulphur (wt. %)	API	Viscosity (cp)
100/0	3.88	24.50	118.80
75/25	2.96	25.54	54.92
60/40	2.44	29.67	32.49
50/50	2.11	28.52	23.39
40/60	1.78	29.85	15.78
25/75	1.00	33.45	5.59
0/100	0.43	38.50	4.98

Sulphur was used as the independent variable and key property of the crude because it has a linear function to the yields generated in the different volumetric ratios Robertson et al. (2011). From the regression plots, the deviated points are not far from the straight line and the reliability for each yield fraction is around 0.9. However, the API and Viscosity from Table 5-1 are highly nonlinear i.e. the lines are not straight, they are rather polynomial. This made the reliability R^2far less than 0.9 details are Appendix E.

5.2.2 The derived regression models for CDU and VDU

The results obtained from the 53runs in Aspen HYSYS on the yield fractions from the different 53 scenarios or volumetric mixing ratios are shown in Figure 5-2 for CDU and VDU.

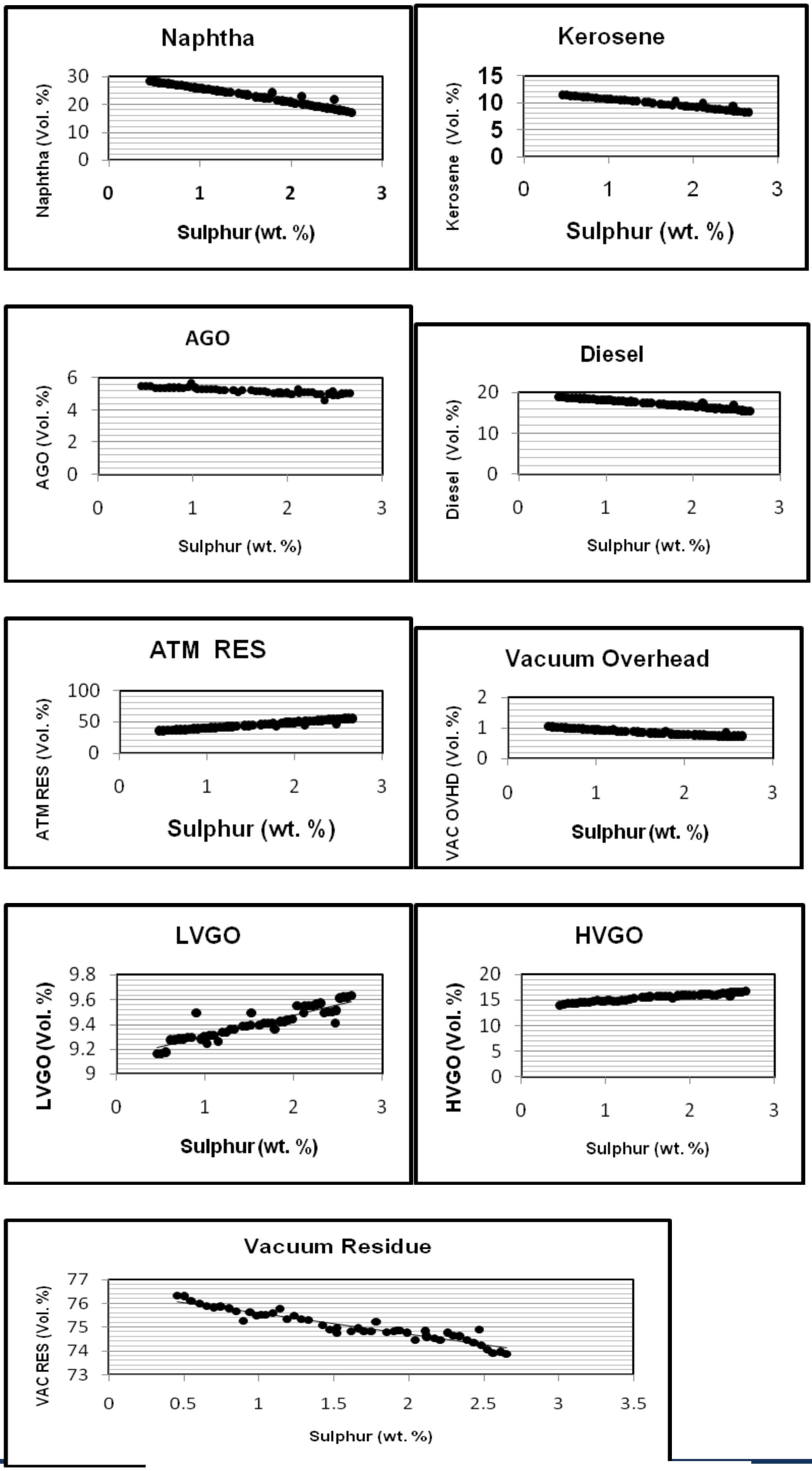

Figure 5-2 Plots of predicted yields from CDU and VDU

The regression model derived for the various CDU and VDU are listed in Table 5-2withthe R^2 which is the confidence level or reliability of the function. The more the $R^2$is close to 1, the lesser the error, the more linear the relationship of Y from X.

These functions are then used as the coefficients for yield prediction in refinery planning for production and products blending subsystem as shown in Table 5-3.

Table 5-2 Regression model derived for CDU and VDU yields

CDU and VDU product Yield	Regression models	R^2
Naphtha	(-4.91 X+ 30.81)	0.9552
Kerosene	(-1.39 X + 12.10)	0.9521
Diesel	(-1.54 X + 19.68)	0.9552
Atmospheric gas oil (AGO)	(-0.25 X + 5.59)	0.7486
Atmospheric Residue	(8.64 X+ 31.49)	0.9603
Low vacuum gas oil (LVGO)	(0.17 X + 9.13)	0.8201
High vacuum gas oil (HVGO)	(1.14 X + 13.66)	0.9477
Vacuum Residue	(-0.89 X + 76.49)	0.9055
Vacuum Overhead	(-0.14 X+ 1.08)	0.9483

Table 5-3 Regression model derived for CDU and VDU units yield

CDU and VDU Yields	Regression model	Coefficients for Regression
Naphtha	(-4.91 X+ 30.81)	$IP_{cdu,f,naphtha,cm}$
Kerosene	(-1.39 X + 12.10)	$IP_{cdu,f,kero,cm}$
Diesel	(-1.54 X + 19.68)	$IP_{cdu,f,diesel,cm}$
AGO	(-0.25 X + 5.59)	$IP_{cdu,f,ago,cm}$
Atm Res.	(8.64 X+ 31.49)	$IP_{cdu,f,atmres,cm}$
LVGO	(0.17 X + 9.13)	$IP_{vdu,f,lvgo,cm}$
HVGO	(1.14 X + 13.66)	$IP_{vdu,f,hvgo,cm}$
Vac Res	(-0.89 X + 76.49)	$IP_{vdu,f,vacres,cm}$
Vac Ovhd	(-0.14 X+ 1.08)	$IP_{vdu,f,vacovhd,cm}$

5.2.3 Validation with GAMS model for CDU and VDU

Some selected volumetric mixing ratios of the crude mix obtained in Aspen HYSYS were run in GAMS using CPLEX solver with the aim of validating the results. The summary of the results were listed in Tables 5-4, 5-5 and 5-6.

Table 5-4 GAMS results for comparison with Aspen HYSYS model

Products	50/50 (Kbbl/day)	25/75 (Kbbl/day)	75/25 (Kbbl/day)	60/40 (Kbbl/day)	40/60 (Kbbl/ day)
Naphtha	22.84	25.73	19.71	21.95	24.07
Kerosene	9.87	10.69	8.95	9.43	10.20
Diesel	17.08	18.09	16.11	16.77	17.50
AGO	5.210	5.39	4.94	5.11	5.34
ATM RES.	44.00	40.09	46.50	46.50	42.88
LVGO	4.138	3.71	4.39	4.67	3.98
HVGO	6.842	5.92	7.40	7.36	7.82
Vac. Ovhd	0.319	0.38	0.37	0.39	0.38
Vac. Res.	32.70	30.08	34.34	33.70	29.85

Table 5-5 Comparison of Yields obtained from GAMS Model and results from AspenHYSYS in 50/50 crude mix.

PRODUCTS	50/50 GAMS		Aspen HYSYS	Difference
	Vol.(Kbbl/day)	Vol. (m^3/h)	Vol. (m^3/h)	%
Naphtha	22.84	155.749	156.60	0.5
Kerosene	9.87	67.3	67.65	0.4
Diesel	17.08	116.47	117.10	0.6
AGO	5.210	35.527	35.70	0.5
ATM RES.	44.00	300.04	308.60	2.5
LVGO	4.138	28.217	29.29	3.4
HVGO	6.842	46.656	48.43	3.7
Vacuum Ovhd	0.319	2.17	2.259	1.3
Vac. Residue	32.70	222.98	231.5	3.6

Table 5-6 Comparison of Yields obtained from GAMS Model and results from AspenHYSYS in 75/525crude mix.

Yields	7 5/25 GAMS		AspenHYSYS	Error
	Vol. (Kbbl/day)	Vol. (m^3/h)	Vol. (m^3/h)	%
Naphtha	19.71	134.4	132.90	0.37
Kerosene	8.95	61.03	60.34	1.1
Diesel	16.11	109.85	108.60	1.1
AGO	4.94	33.68	33.34	1.0
ATM RES.	46.50	317.08	339.10	6.4
LVGO	4.39	30.00	32.38	7.3
HVGO	7.40	50.46	54.62	7.5
Vacuum Ovhd	0.37	2.523	2.711	7.4
Vac. Residue	34.34	234.16	253.4	7.5

From the results shown in Table 5-5 and 5-6, conclusion can the drawn that the values obtained in Aspen HYSYS used to derive regression models in Table 5-1 are good representation of product fractions obtained in CDU and VDU.

5.3 Derivation of regression model for FCC and HDT with information from empirical correlation

During the rigorous modelling of the CDU and VDU in Aspen HYSYS, some of the feed from the CDU and some from the VDU were sent to the FCC. From this information, the inflow into the FCC is known. The feed outflow from the FCC is then calculated using empirical correlations.

The method used for generating the regression model is shown in Appendix C. Table 5-7 is the regression model generated for the FCC unit yield.

Table 5-7 Regression model for FCC

Yields	Regression model	
FCC gas	(-0.85X + 41.77)	$IP_{fcc,f,fccgas,cm}$
TGO	(0.55 X +29.45)	$IP_{fcc,f,tgo,cm}$
Coke	(0.0062 X+3.96)	$IP_{fcc,f,coke,cm}$
C2+lighter	(0.009 X+ 8.28)	$IP_{fcc,f,c2lighter,cm}$
LPG	(0.21 X+16.59)	$IP_{fcc,f,lpg,cm}$

Before the feed enters the FCC, it went through the HDT. For the HDT, the 98% method from Gary and Handwerk (2001) applies.

5.4 Aggregate model development

The detailed regression model derived from the four individual process units are then used to form the aggregate model. The models will not be repeated in this section.

5.5 Refinery production and product blending planning using aggregate model

The regression models derived were used to replace the coefficients in a typical fixed yield in a refinery planning model as obtained in Section 4-1 of 50/50 volumetric ratio. And the results compared.

Case study was performed to verify the efficacy of the model. The same case in Chapter 4 is used in the chapter. The difference is that in the previous chapter, the yield coefficients generated from Aspen HYSYS were used directly as fixed but in this chapter, the regression models derived from the different volumetric ratios and sulphur content in Table 5-3 were used instead.

The refinery planning model outlined in equation 4-19 to 4-33 is used for this case.

5.5.1 Problem statement and implementation

Two crude vessels are expected to arrive with two different sets of crude: Ratawi and Brent. The refinery has one CDU which has been designed to process a capacity of not more than 100,000 barrel per day. The refinery is capable of handling any blend of the two crudes at different proportions. The model since its profit maximization treats the crude oil input and products output as values for the model to determine rather than given. The following are to be determined at the end of the planning horizon:

- Crude input into the CDU
- Quantities of individual products
- Optimal profit
- Which volumetric ratio gave the highest profit
- The sulphur content at that volumetric ratio

5.5.2 Objective function

A planning horizon of 30 days is used for this case study and each day is a time interval. The objective of the optimisation problem is to achieve maximum profit over the entire planning horizon given the type of crude oil and facilities needed in the refinery to produce various products. The cost of purchasing the crude oil and the cost of processing the crude oil is subtracted from the revenue or income generated from the finished products. As stated in equation 4-27.The objective function and all constraints are linear.

5.5.3 Decision variables

The following decision variables have been used in the optimization problem formulation: Flow rates of materials (crude and intermediate) to and from the refinery and the quantities of final products.

5.5.4 Parameters used

The parameters used in this Chapter such as capacity of processing units and product prices are the same as that used in Chapter 4.

5.6 Results and analysis

Table 5-8 Summary of results obtained from the refinery planning model on Aggregate Model

Product Yields	Aggregate Method (Vol. Kbbl)
Naphtha	15.18
Kerosene	7.16
Diesel	13.33
AGO	4.21
ATM RES.	46.5
LVGO	4.46
HVGO	7.76
Vacuum Ovhd	0.32
Vacuum Residue	34.46
FCC-gas	6.36
TGO	4.97
C2+Lighter	1.34
LPG	2.78
FINAL PRODUCTS (kbbl/day)	
GASOLINE BLEND (GB)	21.54
FUEL-OIL	39.44
KEROSENE	7.16
DIESEL	13.33
FUEL-GAS	4.44
PROFIT ($/30 DAYS)	87306

From the results obtained, the highest profit of $87306 was obtained at volumetric ratio of 98% of Ratawi and 2% of Brent crude oil and the sulphur content at this volumetric ratio is 2.655 wt percent. The flow rate of crude into the CDU is about 85,432bbl/day. Implementing the case study with aggregate model, the same volumetric ratio that gave the highest profit in fixed yield method also gave the highest profit in the aggregate model. However, the profit obtained using aggregate model is $87306, and that obtained using fixed yield in Chapter 4 is $84614. The difference in profit is as a result of the quantity of crude oil used in the CDU in both methods. The more the crude used, the more the profit. The quantity of crude used in the fixed yield method is 84,000bbl/day while that used in the aggregate method is 85,432bbl/day.

Table 5-7 is a summary of the results obtained using aggregate model. The volume of intermediates and final produced are listed in the table.

5.7 Comparison between fixed yield method and the regression method

Direct comparison of fixed yield and regression method shows the following detail in Table 5-9.

Table 5-9 Comparing Fixed yield and Aggregate method

Product Yields	Fixed yield method (Vol. Kbbl)	Aggregate Method (Vol. Kbbl)	Relative Error (%)
Naphtha	14.36	15.18	5.4
Kerosene	6.96	7.16	2.7
Diesel	12.99	13.33	2.5
AGO	4.23	4.21	0.5
ATM RES.	46.50	46.5	0.0
LVGO	4.48	4.46	0.5
HVGO	7.81	7.76	0.6
Vacuum Ovhd	0.34	0.32	5.8
Vacuum Residue	34.35	34.46	0.3
FCC-gas	6.36	6.36	0.0
TGO	5.01	4.97	0.8
C2+Lighter	1.35	1.34	0.7
LPG	2.83	2.78	1.8
FINAL PRODUCTS (kbbl/day)			
GASOLINE BLEND (GB)	20.72	21.54	3.8
FUEL-OIL	39.36	39.44	0.2
KEROSENE	6.96	7.16	2.7
DIESEL	12.99	13.33	2.5
FUEL-GAS	4.51	4.44	1.6
PROFIT ($/30 DAYS)	84614	87306	3.0

For direct comparison of fixed yield method and aggregate method, the same case on 98/2 volumetric ratio was used to represent the typical fixed yield and improved method since both gave the highest profit. The results are summarized in Table 5-9. The quantities of final products obtained in fixed yield are the same all through the 30 day planning horizon also the quantities of final products obtained in the aggregate method are the same throughout the 30 day planning horizon also since both cases are deterministic.

The models developed in this chapter are evaluated by comparing the predictions to fixed yield. Since it is evident that the profit $84614obtained for 30 day planning horizon on fixed yield and $87306 for 30 day planning horizon on improved method are close to each other also the flow of intermediates on both approaches are very close and even in some cases like the Atm-res, vacuum residue e .t. care the same so conclusion can then be drawn that he aggregate model can be used for yield estimation or prediction in refinery planning.

The relative percent error between the predicted values from the proposed method and the fixed yield values ranges from 0 to 5.8% as shown in Table 5-9.

5.8 Summary

In this chapter an aggregate model for refinery planning was proposed using regression method. The model was successfully applied for yield prediction in a refinery planning model.

It was discovered that blending of different crude oil changes the properties of the crude. This is evident in Table 5-1. These properties affect the yields obtained from the crude oil.

The procedures are:

- Using the information obtained in Chapter 3 by running 50 times in Aspen HYSYS, regression models were derived for individual products fractions.
- The regression models derived were used in place of the regular fixed yield approach in a mathematical programming model for planning of production and products blending subsystem. The results obtained from the two methods were compared.

The aggregate model provided a better approach for yield estimate; it is more convenient than the regular fixed yield approach. The main differences between the two approaches are:

- For the fixed yield method, the rigorous modelling was carried out 50 times on different volumetric mixing ratios and the mathematical programming was also carried out 50 times for individual volumetric mixing ratios before being able to determine the volumetric ratio that gave the highest profit.
- For the aggregate model, the rigorous modelling was carried out 50 times, the values were then used to generate linear functions which were then used to carry out only one run of the mathematical programming to find the highest profit.
- The predicted data by the aggregate model is close to that obtained by fixed yield method. Conclusion can be drawn that regression model can be used to predicts yields in refinery production and product blending subsystem planning.

6 Planning for the Integrated Refinery Subsystems under Deterministic Condition

6.1 Introduction

This chapter is aimed to deal with tactical planning for the integrated refinery subsystems with MILP under deterministic condition. In this work, the three main subsystems of a refinery are integrated under deterministic conditions. These include crude unloading, production and product blending, and product distribution subsystems. The profit is maximized considering the revenue from the products, raw material costs, inventory costs, transportation costs, and operation costs. A case study is used to demonstrate the applicability of the proposed model and solution approach.

The refinery subsystems models for integration considered in this work include the following:

- The modified scheduling model for crude unloading subsystem by Lee et al. (1996)
- The aggregate model for production and product blending subsystem developed in Chapter 5 of this Thesis.
- A planning model for product distribution by Alabi and Castro (2009)

The following assumptions are considered:

- Quantity of crude oil remaining in the pipe is neglected
- The mass balance on yields of individual process (i.e. CDU, FCC e.t.c.) units is used to determine the product flow rates, which are also function of the feed.

6.2 Planning model for the crude unloading subsystem

In this subsystem,

- The short term scheduling model presented in Lee et al. (1996) was modified for planning purposes.
- The planning horizon is 30 days
- The bilinear term for component balance is not considered

Given the following parameters:

- Waiting time of each vessel in the sea
- Unloading duration time for each vessel
- Crude unloading rate from vessels to storage tanks
- Crude oil transfer rate from the mixing tank to CDU
- Inventory levels of storage tank (Lee et al. 1996)

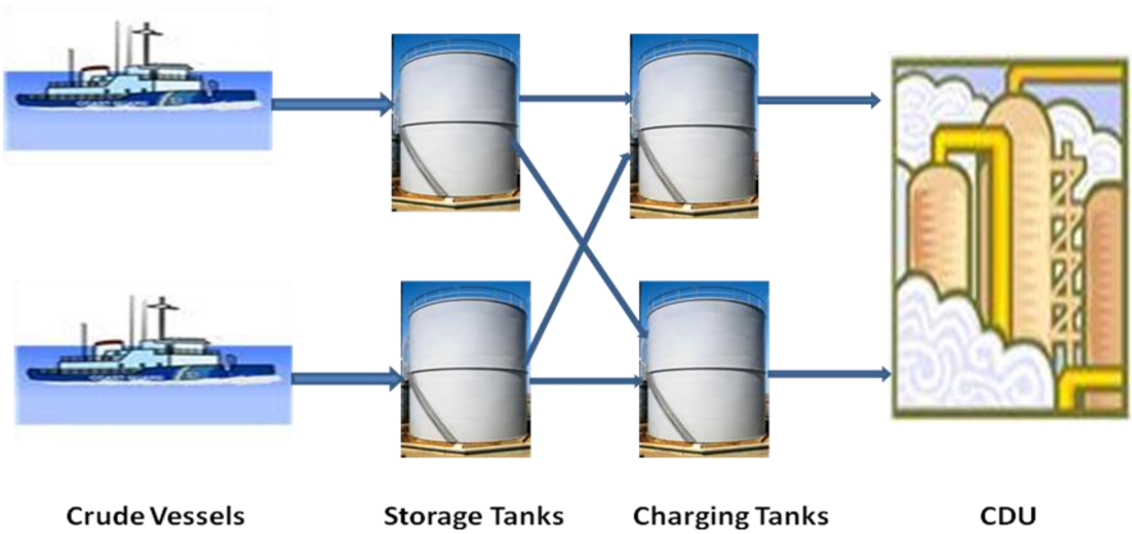

Figure 6-1 Flow of crude oil for Crude unloading subsystem

The following operating rules must be obeyed in this problem:

- Each vessel should turn up and depart from the docking station for crude oil discharge within the planning horizon.
- A vessel can only unload its crude oil if it arrives at the dock station.
- If a vessel leaves the docking station, it cannot unload the crude oil.

- The vessel should leave the docking station after its arrival.
- The vessel cannot arrive at the docking station if the preceding vessel does not leave.
- Crude oil cannot be fed into the mixing tank that is feeding the CDU.
- CDU receives one mixed crude at time interval.

6.2.1 Mathematical model formulation for crude unloading subsystem

Vessel operations rule

A vessel arrival at the ducking station once within the horizon

$$\sum_{t=1}^{T} XF_{v,t} = 1, \forall\ v \in VE \qquad (6-1)$$

Each vessel is allowed to leave once all through the horizon

$$\sum_{t=1}^{T} XL_{v,t} = 1, \forall\ v \in VE \qquad (6-2)$$

Each unloading activity begins

$$TF_v \sum_{t=1}^{T} tXF_{v,t} = 1, \forall\ v \in VE \qquad (6-3)$$

Each unloading activity ends

$$TL_v \sum_{t=1}^{T} tXL_{v,t} = 1, \forall\ v \in VE \qquad (6-4)$$

Each vessels unloads as soon as it arrives as set by the planners

$$TF_v \geq TARR_v \qquad \forall\, v \in VE \qquad (6-5)$$

Unloading duration is thus,

$$TL_v - TF_v \;\geq 1 \qquad \forall\, v \in VE \qquad (6-6)$$

The initial vessel must complete unloading its contents one time interval before the ensuing vessel comes for unloading.

$$TF_{v+1} \geq TL_v + 1 \qquad \forall\, v \in VE \qquad (6-7)$$

The possible time periods for unloading to occur is between time TF_v and TL_v

$$KY_{v,i,t} \leq \sum_{t=1}^{T} XF_{v,t} \quad \forall\, v \in VE, \forall\, t < m, \forall m \in \{TARR_{v,\ldots,}TDP_v\} \qquad (6-8)$$

$$KY_{v,i,t} \leq \sum_{t=1}^{T} XL_{v,t} \quad \forall\, v \in VE, \forall\, t > m, \forall m \in \{TARR_{v,\ldots,}TDP_v\} \qquad (6-9)$$

Flow in and out of storage tank cannot occur simultaneously

$$KYS_{i,j,t} \leq 1 - KY_{v,i,t} \forall\, v \in VE, \forall i \in ST, \forall j \in CT \qquad (6-10)$$

6.2.2 Material balance equations for the vessel:

Crude oil in vessel v at time t is equal to initial crude oil in the vessel v minus crude oil transferred from vessel v to storage tank i up to time t.

$$VV_{v,t+1} = VV_{v,t} - \sum_{i=1}^{I} FVS_{v,i,t} \quad \forall v \in VE, \qquad \forall t \in T \qquad (6-11)$$

Operating constraints on crude oil transfer rate from vessel v to storage tank i, at time t.

$$FVS_{v,i,tmin} \times KY_{v,i,t} \leq FVS_{v,i,tmax} \times KY_{v,i,t} \ \forall v \in VE, \forall i \in ST, \qquad \forall t \in T \qquad (6-12)$$

In an event where there are more vessels than the available storage tanks, the storage tanks are still used for the mixing operation.

$$FVS_{v,i,tmin}\left(1 - F_{i,j,t}\right) \leq FVS_{v,i,t} \leq FVS_{v,i,tmax}\left(1 - F_{i,j,t}\right) \forall v \in VE, \forall i \in ST, \quad \forall t \in T \qquad (6-13)$$

The volume of crude oil transferred from vessels v to storage tank during the time horizon equals the initial crude oil volume of vessel, v.

$$\sum_{i=1}^{I} \sum_{t=1}^{T} FVS_{v,i,t} = VV_{v,t} \ \forall v \in VE, \qquad t = 0 \qquad (6-14)$$

6.2.3 Material balance equations for the storage tanks:

The crude oil in storage tank i at time t equal to initial crude oil in storage tank i plus crude oil transferred from vessels to storage tank i, up to time t minus crude oil transferred from storage tank i, to charging tanks j up to time t:

$$VS_{i,t+1} = VS_{i,t} + \sum_{v=1}^{V} FVS_{v,i,t} - \sum_{j=1}^{J} FSB_{i,j,t} \quad \forall i \in ST, \forall t \in T \qquad (6-15)$$

Operating constraints on crude oil transfer rate from storage tank i to charging tank j at time t.

$$FSB_{i,j,t} \times KYS_{i,j,t} \leq FSBmax_{i,j,t} \times KYS_{i,j,t}, \quad \forall i \in ST, \forall j \in CT, \forall l \in CDU, \forall t \in T \ (6-16)$$

Volume capacity limitations for storage tank i:

$$VSmin_i \leq VS_{i,t} \leq VSmax_i, \qquad \forall i \in ST, \qquad \forall t \in T \qquad (6-17)$$

6.2.4 Material balance equations for charging tank:

Crude oil mix in charging tank j at time t equal to initial mixed oil in charging tank j plus crude oil transferred from storage tanks to charging tanks j up to time t minus crude oil mix j charged into CDU l up to time t:

$$VB_{j,t+1} = VB_{j,t} + \sum_{i=1}^{I} FSB_{i,j,t} - \sum_{l=1}^{L} FBC_{j,l,t}, \qquad \forall j \in CT, \qquad \forall t \in T \qquad (6-18)$$

Operating Constraints on mixed oil transfer rate from charging tank j to CDU l at time t:

$$FBC_{j,l,t} \times KYB_{j,l,t} \leq FBCmax_{j,l,t} \times KYB_{j,l,t} \quad \forall j \in CT \quad \forall l \in CDU, \forall t \in T \qquad (6-19)$$

Volume capacity limitations for charging tank *j* at time *t:*

$$VBmin_j \leq VB_{j,t} \leq VBmax_j \quad \forall j \in CT, \forall t \in T \qquad (6-20)$$

The flow rate (PC) of mixed crude entering the CDU *l* at time t, is the sum of the individual crude oil entering the charging tank ($\sum_{l=1}^{L} FBC_{j,l,t}$).

$$\sum_{j,l} FBC_{j,lt} = PC_{cm,t} \quad \forall J \in j, cm \in CM \qquad (6-21)$$

At this point, the yields obtained in the CDU are a function of the type of crude mix, the property (sulphur in the crude mix) and flow rate of the crude mix.

$$IP_{u,f,f',cm,t} = Prop_{cm,t} \qquad (6-22)$$

6.2.5 Rules that must be followed for charging of crude oil during operation

The charging tank j is allowed to feed at most one CDU l at any time interval.

$$\sum_{i=1}^{L} \mathrm{KYB}_{j,l,t} \leq 1 \qquad (6-23)$$

CDU l can only receive charged crude oil from one charging tank j at any time interval.

$$\sum_{j=1}^{CT} \mathrm{KYB}_{j,l,t} \leq 1 \qquad (6-24)$$

Changeover penalty: If CDU *l* is fed by crude oil mix *j,* at time *t* and later changed from crude tank *j* to *j'* changeover is incurred. This is defined by Lee et al. (1996).

$$Z_{j,g,l,t} \geq KYB_{j,l,t+1} + D_{j,l,t} - 1 \qquad (6-25)$$

$$j, g(j \neq g) \in CT, \forall l \in CDU$$

$$D_{j,l,t} = KYB_{j,l,t} \qquad (6-26)$$

Set up penalty: When vessels are allowed to stand for brine settling, in other to start further unloading and transfers, cost is incurred. For this reason a set up penalty has been included in the model. This penalty is for any period any tank is allowed to stand.

$$\left(\sum_{t=1}^{T} \sum_{i=1}^{ST} \mathrm{XR}_{i,t}\right) \times \mathrm{PMD} \qquad (6-27)$$

This is included in the objective function.

Information in Table 6-1 is used for the crude unloading subsystem

Table 6-1 Data used for the 30 day horizon (Lee et al., 1996)

Planning Horizon (# of unit Time)			30days Period
Number of Vessels Arrivals			2
	Arrival Time	Amount of Crude Oil	Sulphur Content
Vessel 1	Period 1	1,500,000/ bbl	0.0043
Vessel 2	Period 16	1,500,000 /bbl	0.0388
Number of Storage Tank		2	
Storage Tanks	Max Capacity	Initial oil Amount	
Tank 1	1,500,000/bbl	250,000 bbl	
Tank 2	1,500,000/bbl	750,000 bbl	
Number of Charging Tanks		2	
Charging Tanks	Max Capacity	Initial oil Amount	Sulphur content
Tank 1	1,500,000/ bbl	100,000/ bbl	(0.0043)
Tank 2	1,500,000/ bbl	100,000/ bbl	(0.0388)
Number of CDU		1	
Maximum flow from vessel to storage			100,000bbl/period
Maximum flow from one storage tank to charging tanks			100,000bbl/ period
Cost involved in Vessel operation		Unloading: US$8,000/ period Sea waiting US$5,000/ period	
Tank Inventory Cost		Storage Tank: US$ 0.005/(period x bbl) Charging Tank: US$ 0. 008/(period x bbl)	
Crude Oil Demand		100,000bbl/ period	

6.3 Planning model for the production and product blending subsystem

The planning model for this subsystem is the planning model for mixed crude developed in Chapter 5 of this thesis. The refinery topology used in that same chapter applies to this also. The CDU, VDU, FCC and HDT process model in equation 4-19 to 4-31 is used. This relates to the properties of the feed stream as well as operating variables. Normally, mass balances and yield expressions are used to determine products flow rates.

6.4 Planning model for the products distribution subsystem

The model presented in Alabi and Castro (2009) is adopted. Final products from the blending headers are stored in corresponding product tanks from where the products are transported to different depots. In this subsystem, the following constraints are applicable.

Mathematical model formulation for product distribution subsystem

Inventory cost of the product tank:

The total inventory cost of the product tanks at time t is equal to the sum of all the volume of final product in the product tank multiply by the unit cost of inventory of the product tank.

$$CINVPT_t = \sum_{(fp,pt) \in FP,PT} V9_{fp,pt,t} \times cinv3_{pt} \forall_t \qquad (6-28)$$

Product tank capacity limitations:

The volume of final products in the product tanks is less than maximum capacity of the product tank and greater than the minimum capacity of the products tanks.

$$\sum_{fp \in FP (fp,pt) \in FPPT} V9_{fp,pt,t} \leq vmax_{pt} \forall_{pt,t} \quad (6-29)$$

$$\sum_{fp \in FP (fp,pt) \in FPPT} V9_{fp,pt,t} \geq vmin_{pt} \forall_{pt,t} \quad (6-30)$$

Flow Limitations

Flow of final product equal to the flow of final product to the depot at time t:

$$FFP_{fp,t} = F8_{fp,pt,dp,t} \ \forall_{fp,pt,dp,t} \quad (6-31)$$

Flow of final product to the depot satisfies the demand at the depot

$$F8_{fp,pt,dp,t} = DEM1_{fp,pt,dp,t} \forall_{fp,pt,dp,t} \quad (6-32)$$

Material balance of final product in the product tanks at time t:

The volume of final product fp in the product tank pt at time t is equal to the initial volume of product in the product tank pt plus flow of product to the depot minus the demand of final product by the depot.

$$V9_{fp,pt,t} = V04_{fp,pt} + F9_{fp,pt,t} - DEM_{fp,pt,t} \quad (6-33)$$

Transport cost of final product to the depot at time period t

The total transport cost of final product to the depot at time t is equal to the sum of flow of final product to the depot multiply by the unit cost of transportation of the final products to the depot.

$$CTR_t = \sum_{(fp,pt,dp,t) \in FPPTDP} F8_{fp,pt,dp,t} \times CT_{fp} \forall_t \quad (6-34)$$

Depot mass balance for final product at time period t

The quantity of final products in the depot is equal to the initial volume of final product in the depot multiply by the sum of flow of final products into the depot

$$VFPDP_{dp,t} = VIDP_{dp} + \sum_{fp} F8_{fp,pt,dp,t} \forall_t \qquad (6-35)$$

6.5 Planning model for the integrated refinery subsystems

In this section, the planning model developed for the individual subsystems are being integrated and used in a refinery planning.

For the model to be feasible the production and product blending subsystem was first solved and the requirement of the CDU was then passed to the crude oil unloading subsystem.

The bilinear terms is avoided in this thesis.

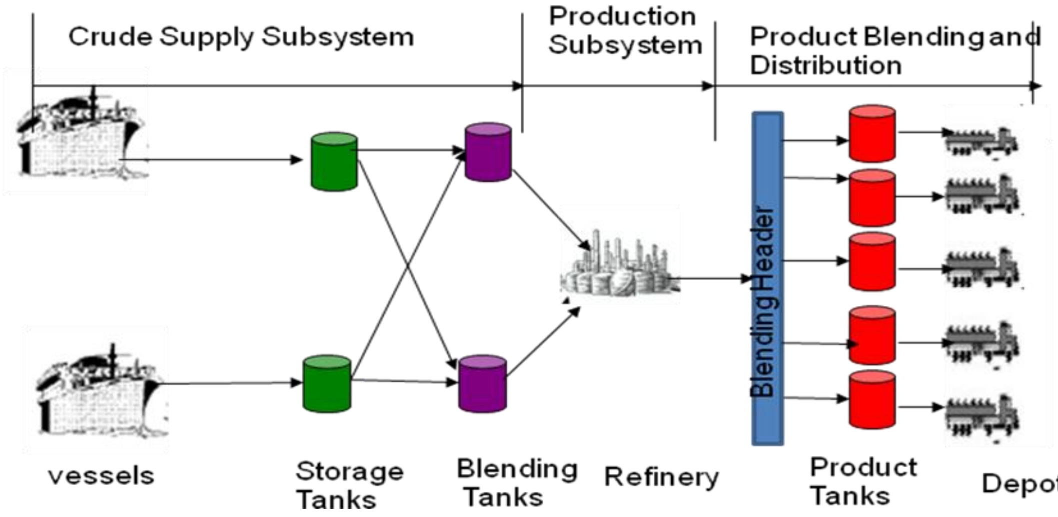

Figure 6-2 Schematics for the Integrated Refinery Subsystems

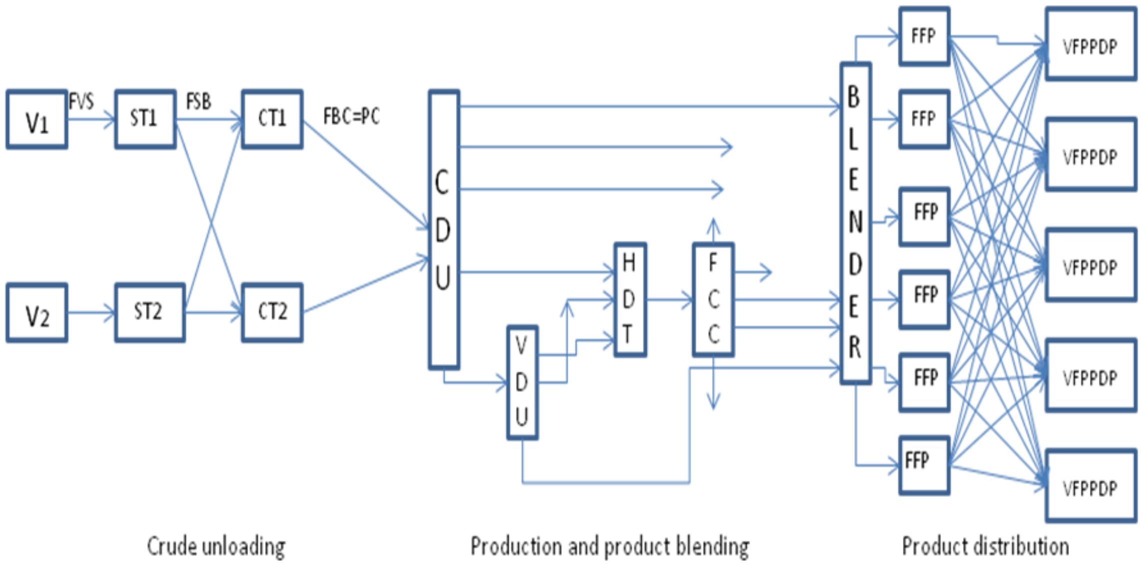

Figure 6-3 Schematics for the Integrated Refinery Subsystems

6.6 Refinery planning for integrated subsystems

Because it is deterministic, the cost of crude oil and products demand do not vary all through the planning horizon.

Material balance for crude mix

$$\sum_{u \in U} IP_{u,f,f'cm} \times PROLEV_{u,cm,t} + PC_{cm,t} \geq 0 \qquad (6-36)$$

Capacity constraint

The capacity of the process units is at all times greater than the sum of all the feed stream flows into it.

$$\sum_{cm \in CM} PROLEV_{u,cm,t} \leq cap_u \forall_{u,t} \qquad (6-37)$$

Material balance for intermediates

The coefficients of the intermediate fractions multiply by the level of the process and the flow of intermediate materials that are purchased from the third party

(Butane) are greater than the total intermediate material that are blended into final products.

$$IP_{u,intm,cm} \times PROLEV_{u,cm,t} + FM_{intm,cm,t} | intm \in pmat \geq \sum_{(fp,intm) \in BL} BLINT_{cm,intm,fp,t} \quad \forall intm, b, t \qquad (6-38)$$

Final products constraint

The flow rate of individual final products is equal to intermediate final products that reach blending

$$FFP_{fp,t} = \sum_{(fp,intm) \in blnposs, cm \in CM} \sum BLINT_{cm,intm,fp,t} \, \forall_{fp,t} \qquad (6-39)$$

Quality constraint

Quality attribute (i.e. specifications) for the products must be less than maximum and greater than minimum specifications. These are represented in Equation (6-40) and (6-41).

$$\sum_{intm \in INTM \setminus (fp,intm) \in BL, cm \in CM} \sum prop\_fp_{intm,cm,q} \times BLINT_{cm,intm,fp,t} \geq PropMINFP_{fp,q} \times FFP_{fp,t} \quad \forall (fp), t, q \setminus propMINFP_{fp,q} \neq 0 \qquad (6-40)$$

$$\sum_{intm \in INTM \setminus (fp,intm) \in BL, b \in B} \sum prop\_fp_{intm,cm,q} \times BLINT_{b,intm,fp,t} \leq propMAXFP_{fp,q} \times FFP_{fp,t} \quad \forall (fp), t, q \setminus propMAXFP_{fp,q} \neq 0 \qquad (6-41)$$

Crude mix cost and cost of all purchased intermediates

The cost of crude oil mix and the cost of intermediate materials e.g. butane form the input material cost.

$$IMPCST_t = \sum_{pmat \in PMAT} \sum Cost2_{pmat,t} \times \sum_{cm \in CM} \sum Cost1_{cm,t} \times PC_{cm,t} \qquad (6-42)$$

Cost of operation

The cost of all the refinery units multiply by the level of the process makes up the cost of the refinery operations.

$$COP_t = \sum_{u \in U} \left(Cost_u \times \sum PROLEV_{u,cm,t} \right) \qquad \forall t \qquad (6-43)$$

Total income

This is the total revenue generated from sales of the final products and its represented in Equation (6-44).

$$REV_t = \sum \sum_{fp \in FP} RV_{fp} \times FFP_{fp} \qquad \forall t \qquad (6-44)$$

6.6.1 Problem statement and implementation

Two crude vessels are expected to arrive with two different sets of crude: Ratawi and Brent. The refinery has one CDU which has been designed to process a capacity of not more than 100,000 barrel per day. The refinery is capable of handling any blend of the two crudes at different proportions. In this case, the product price, the process capacities are the same as in chapter 5 of this thesis. The model since its profit maximization treats the crude oil input and products output as values for the model to determine rather than given.

6.6.2 Objective function

A planning horizon of 30 days is used for this case study and each day is a time interval.

$$\sum_{t\in T} REV_t - \sum_{t\in T} COP_t - \sum_{t\in T} IMPCST_t - CINVST\sum_{i=1}^{I}\sum_{t=1}^{T}(VS_{i,t} + VS_{i,t+1}|2)$$

$$- \mathrm{CUNLD}_{\mathrm{v}}\sum_{\mathrm{v}=1}^{\mathrm{VE}}[(\mathrm{TL_v} - \mathrm{TF_v}) + 1] - \mathrm{CSEA}_{\mathrm{v}}\sum_{\mathrm{v}=1}^{\mathrm{VE}}(\mathrm{TF_v} - \mathrm{TARR_v})$$

$$- \sum_{t\in T} CTR_t - \sum_{t\in T} CINVPT_t - \sum_{\mathrm{t}=1}^{\mathrm{T}}\sum_{\mathrm{j}=1}^{\mathrm{CT}}\sum_{\mathrm{g}=1}^{\mathrm{CT}}\sum_{\mathrm{l}=1}^{\mathrm{L}}(\mathrm{CSETUP_{j,g,l}}\,\mathrm{Z_{j,g,l,t}})$$

$$- \left(\sum_{\mathrm{t}=1}^{\mathrm{T}}\sum_{\mathrm{i}=1}^{\mathrm{ST}}\mathrm{XR_{i,t}}\right) \times \mathrm{PMD} \qquad (6-45)$$

The objective function for the integrated refinery subsystem is to maximize the profit of the refinery, defined as the sales revenue *(REV),* minus the cost of refining *(COP),* the cost of feed *(IMPCST),* minus total operating cost which is unloading cost *(CUNLOAD),* storage tank inventory cost *(CINVST),* sea waiting cost *(CSEA),* transport cost *(CTR),* product tank inventory cost *(CINVPT),* changeover cost *(CSETUP)* and penalty cost *(PMD).*

6.6.3 Decision variables

The following decision variables have been used in the optimization problem formulation: Flow rates of materials (crude and intermediate) to and from the refinery, what is the volumetric mixing ratio that yielded the profit and the quantities of final products.

6.6.4 Parameters used

Same as Chapter 5 for the production and product blending subsystem, and Information for crude unloading is in Table 6-1.

Table 6-2 Final products quality specification (AMD Refinery data)

	Octane	VP (mmHg)	Density kg/m³	Sulphur (wt . fraction)
GB	>86			0.002
GB	<90	9.0		0.002
Kerosene				0.0015
Diesel				0.005
Fuel-gas			860	0.005
fuel-oil			1100	0.04

6.7 Results and analysis

The case study was implemented in GAMS and optimized with CPLEX solver. The optimal profit of $75, 954 was obtained in 1.25 second after 1364 iterations. This contains 6,367 variables, 9,625 equations and 397 discrete variables as shown in Table 6-3. Figure 6-3 shows the summary of the amount of final products produced. Vessel 1 arrived on the first day and finished unloading on day 15, while vessel 2 arrived on day 16 and finished unloading on day 29.

Table 6-3 Summary of results for the integrated refinery subsystem

Planning horizon	30
Equations	**9,625**
Variables	**6,397**
Discrete variables	**397**
Objective Function$/30days	**75954**

The profit for the integrated subsystem $75,954came down compared to $87,306 obtained from the production and products blending subsystem, because the cost items such as unloading, inventory etc. Cost in the crude unloading subsystem and the cost in the product distribution subsystem were considered realistically. The total quantity of crude purchased is 3,000,000bbl for the planning horizon. The refinery made use of the cheaper crude more than the expensive crude.

1,720,000bbl of crude type 1 (Ratawi) was used compared to 1,280,000bbl of crude type 2 (Brent) used during the entire planning horizon. The reason is that Ratawi crude is cheaper crude than Brent. The volumetric mixing ratio of 57% of Ratawi and 43% of Brent was used for the refinery operation to be profitable.

For the refinery operation to be profitable, more of the cheaper crude was used than the more expensive one.

Though assumption was made that the processing cost of the crude no matter the volumetric mix has the same cost of operation, this is not always the case in real refinery process.

The CDU feed flow rate increased to100,000bbl/day compared to the feed rate of non- integrated subsystem (85,432bbl/day), this is because the CDU is trying to maximise the crude consumption for profit to be maximised. The CDU maximum capacity is 100,000bbl/day.

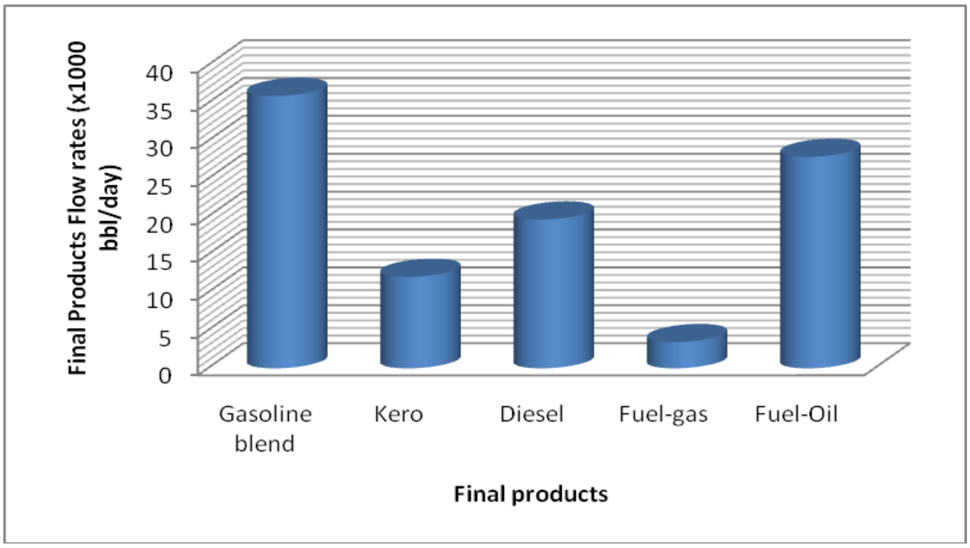

Figure 6-3 Flow rate of Final Products

From Figure 6-3, the production of gasoline blend is more followed by the production of fuel-oil. The production of Fuel-gas has the least product flow rate. The quantity of gasoline blend increased due to the increased quantity of crude type two compared to the quantity produced in the non-integrated subsystems.

The reason why the refinery made use of the stated volumetric ratio 57% and 43% of the two crudes in this integrated subsystem compared with the 98% and 2% obtained in the non-integrated subsystem are:

- The raw material cost and the products price in the two models are the same, and there are more cost functions to be considered e.g. cost of inventories and unloading, sea waiting costs and other constraints, so the system has to optimally operate to maximise profit.
- From the flow of final products for the non-integrated subsystem in Table 5-8, the quantity of fuel-oil produced is more than the quantity of gasoline blend produced because there are more of the cheaper crude than the expensive crude and less constraints. But in the integrated subsystem, the reverse is the case, this is because, the system observed that there are more constraints and also from the market requirement, there is a chance of producing more gasoline blend which has a higher market value than fuel-oil and this will boost the refinery profit. To produce the gasoline blend, the refinery requires appreciable quantity of the expensive crude; this made the use of crude type two or the expensive crude to increase from 2% to 43%. Also the quantity of other products e.g. kerosene, diesel increased in the integrated subsystem.

The use of this volumetric mixing ratio affected the capacities of the process units e.g. CDU, VDU and FCC. The CDU was maximally utilised while the VDU because of the higher quantity of crude type two, it brought down the capacity utilization from 46.5 to 31.67kbbl/day.

6.7.1 Variation in Crude oil Price

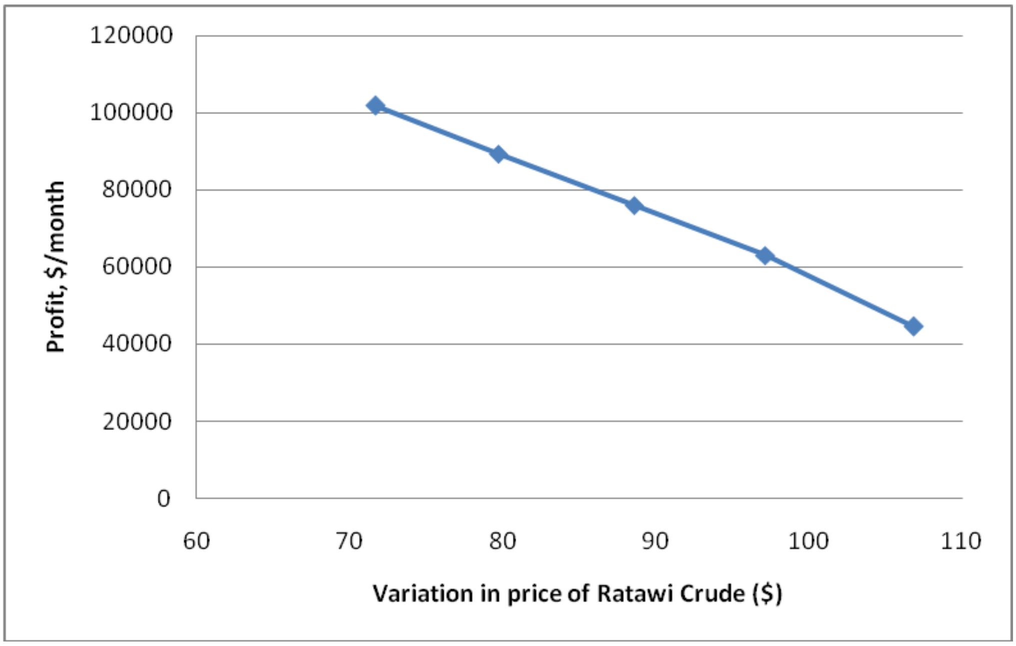

Figure 6-4 Refinery Profit and Variation in crude Price

Figure 6-4 shows how variation in crude price could affect the profit of a refinery. Ratawi crude was used as an example in this case. The Figure shows that if there is an increase or decrease in crude oil price, it will reflect in the profit of the refinery. This also explains the effect of crude price on refinery margin as stated in the motivation of this thesis. It is confirmed that crude price is up to 80% of the refinery profit margin is true. This is in agreement with Arofonosky et al (1978).

The variation in price of ratawi crude only is stated in this thesis because both crude types showed the same trend.

6.7.2 Variation in Final Products Price

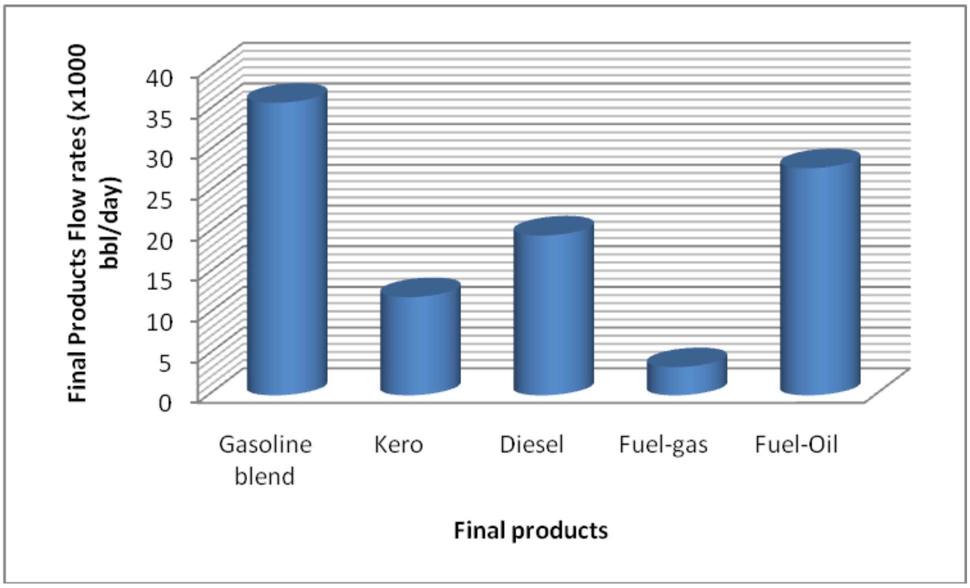

Figure 6-5 Variation in Final product Price

Figure 6-5 shows a variation in the final products price by 10%. 10% increase in products prices increased the final products flow rate and this also increases the profit margin of the refinery from $75,954to $114,223. Increase in products prices happens when there is scarcity of a particular product and also it could happen when there is increase in raw material cost.

6.8 Summary

In this chapter, the three model for the three basic refinery subsystems were joined together as one to form an integrated model and its then used for refinery planning. In the integrated refinery case study result, it was discovered that the system made use of more crude, but gave a lesser profit compared with the non-integrated systems. This is because there are more cost function from the crude unloading and products distribution subsystems taking from the production and products blending subsystem. Variation in crude oil price and variation in final product price were also carried out and the results obtained.

7 Conclusions and Recommendations for Future Work

7.1 Conclusions

This work studies the tactical planning for the integrated refinery subsystems using MILP as the optimization technique.

Recent advances in the modelling of process units for refinery planning and scheduling were reviewed, revealing the current gaps in knowledge. In particular it was observed that the trend has been the use of mixed crude for refinery planning and that crude mix has not yet being reported using the proposed method. There is no existing model on planning of the integrated subsystems of the refinery.

7.1.1 Rigorous modelling of CDU and VDU

The CDU and VDU were rigorously modelled in Aspen HYSYS and the yields obtained from the CDU were validated with data from literature. The CDU alone was validated because there is no case in the literature to validate the VDU yield results with. Process analyses were further carried out on some of the scenarios or volumetric mixing ratios. It was observed that the yields from the CDU match with what is obtained in the literature.

7.1.2 Fixed yield method for refinery production and product blending subsystem planning

The information from the rigorous modelling on CDU and VDU were then transferred into simplified CDU and VDU model for planning. The FCC and HDT units that were derived by correlations were also transferred into simplified FCC and HDT model for planning.

About 53 runs for different scenarios or volumetric mixing ratios were carried out in the rigorous model developed. The simplified model for the process units were then used to run 53 mathematical model for the individual volumetric mixing ratios using fixed yield method with the aim of determining the volumetric mixing ratio that has the highest profit and the sulphur content at that volumetric mixing ratio. At the end, the volumetric mixing ratio that has the highest profit was determined to be blending ratio of 98% of Ratawi crude and 2% of Brent crude and the profit obtained was $84614 at 2.655 wt. percent of sulphur.

7.1.3 Aggregate model for refinery production and product blending subsystem planning

An aggregate model for the production and products blending subsystem of a refinery was developed using regression method and used on the same case study as in the fixed approach. For the aggregate model to be derived, information was transferred from the rigorous model to mathematical programming model and used as fixed yield approach and later regressed linearly and used. However, in using the aggregate model developed in determining the volumetric mixing ratio that yields the highest profit, a single run of the mathematical programming model was carried out compared to the 53 runs in regular fixed yield counterpart. The model developed serves as an alternative approach to calculating the yield in the process units for refinery planning. The profit obtained in aggregate method is $87306 and at the same volumetric ratio and sulphur content as the fixed yield method.

7.1.4 Planning for the integrated refinery subsystems

Three models were integrated together to develop a refinery planning model for the three refinery subsystems which are the crude unloading subsystem, the production and products blending subsystem and the products distribution subsystem.

The aggregate model developed for the production and products blending subsystem, the modified Lee et al.(1996) model for scheduling the crude unloading subsystem and the product distribution model developed by Alabi and Castro (2009) were integrated into a refinery planning model and a case study implemented. After solving the case study, it was discovered that the profit obtained reduced to $75,954 and at a volumetric ratio of 57% of Ratawi and 43% of Brent.

7.2 Recommendations for future work

7.2.1 Consideration of more than two pre-mixed crude oils

For the aggregate model developed, two crude oils were mixed together, there is also the need to consider the mix of more than two different crude oils and their properties like the API and the viscosity incorporated in the regression technique and solves using nonlinear regression model.

7.2.2 Validation of CDU model

In this work the CDU model was validated alone due to lack of data for benchmark, there is need for the VDU to be validated as well. Also more detailed modelling of HDT and FCC should be carried out

7.2.3 Consideration of uncertainty

This model assumed certainty in the yield from the various processes, which may not always the case. On this note uncertainty in the yield should be carried out.

Planning of the supply chain under uncertainty is very crucial due to the changing market conditions and the existence of lead times i.e. difference between the time an order is put and the delivery time in supply chain, the variables for production need to be determined prior to the realisation of demand. There is need to incorporate uncertainty in the integrated model.

7.2.4 Real life case study for Refinery Planning

Some of the data used for the case study were assumed; therefore the model should be used on a complete and real refinery data to confirm the efficacy. In Chapter 4 and 5 of this Thesis, assumption was made that the operating cost for all the volumetric mixing ratios are the same which in real life situation, more sulphur in the crude oil, may increases the operating cost. Some real life data should be used to implement the idea.

Most of the refinery operations has a range of sulphur specification that the CDU has been designed to handle, the regression would have to fall within the specification range. The recent CDU's are designed to be robust and is able to handle wider range of crude oil types. In this case, the regression model would be wide and should fall within range.

In this work sulphur only was considered, it will be good if other crude properties like viscosity API etc. are considered when developing the regression model.

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Appendices

Appendix A (Ratawi and Brent Crude Assay)

The crude assays were used to characterise the crude for rigorous modelling. The crude assay was entered in the oil environment of Aspen HYSYS for the individual crude. These assays will give the simulation model the estimated volume percent of the liquid to be distilled at a given temperature. The rigorous modelling was carried out in the Chapter 3 of this Thesis.

RATAWI - SUMMARY OF MAJOR CUTS

	Whole Crude	Light Naphtha	Medium Naphtha	Heavy Naphtha	Kero	Atm Gas Oil	Light VGO	Heavy VGO	Vacuum Resid	Atm Resid
TBP Temp At Start, °C	Start	10	80	150	200	260	340	450	570	340
TBP Temp At End, °C	End	80	150	200	260	340	450	570	End	End
TBP Temp At Start, °F	Start	55	175	300	400	500	650	850	1050	650
TBP Temp At End, °F	End	175	300	400	500	650	850	1050	End	End
Yield at Start, vol%		1.7	5.6	15.3	21.0	29.2	40.4	57.3	71.5	40.4
Yield at End, vol%		5.6	15.3	21.0	29.2	40.4	57.3	71.5	100.0	100.0
Yield of Cut (wt% of Crude)		2.8	8.0	5.0	7.4	10.6	17.2	15.0	32.9	65.1
Yield of Cut (vol% of Crude)		3.9	9.7	5.8	8.2	11.2	16.9	14.2	28.5	59.6
Gravity, °API	24.5	82.9	57.0	49.3	41.4	33.2	22.1	15.7	3.5	11.2
Specific Gravity	0.9068	0.6601	0.7507	0.7828	0.8182	0.8592	0.9210	0.9615	1.0482	0.9914
Sulfur, wt%	3.88	0.01	0.08	0.33	0.98	2.42	3.50	4.20	6.96	5.41
Mercaptan Sulfur, ppm		274	597	258	72	29	8	0		
Nitrogen, ppm	2066		0	0	1	90	759	1528	5156	3158
Hydrogen, wt%	11.7	16.2	14.3	14.3	13.7	13.0	12.0	11.1	9.2	10.4
Viscosity @ 40 °C (104 °F), cSt	30.5			1.13	1.78	5.87	27.0	272	1.10E+09	4102
Viscosity @ 50 °C (122 °F), cSt	21.5			0.982	1.51	4.40	17.7	143	6.13E+07	1750
Viscosity @ 100 °C (212 °F), cSt	6.19			0.576	0.824	1.59	4.18	17.5	32200	115
Viscosity @ 135 °C (275 °F), cSt	3.52			0.443	0.613	0.996	2.23	7.33	2660	37.9
Freeze Point, °C				-60.000	-38.000	-4.000	27.0			
Freeze Point, °F				-76	-36	25	81			
Pour Point, °C	-23			-68	-41	-6	24	41	40	22
Pour Point, °F	-10			-90	-42	22	76	106	104	72
Smoke Point, mm (ASTM)				28	23	18				
Aniline Point, °C			52	57	61	68	73	78		
Aniline Point, °F			125	135	142	154	164	173		
Total Acid Number, mg KOH/g	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1		
Cetane Index, ASTM D976				43	48	49				
Diesel Index			71	66	59	51	36	27		
Characterization Factor (K Factor)	11.8	12.8	11.8	12.0	11.8	11.8	11.6	11.7	11.5	11.6
Research Octane Number, Clear		68.1	51.0	18.6						
Motor Octane Number, Clear		66.5	48.9							
Paraffins, vol%		85.7	57.7	62.1	46.8	43.5	29.0			
Naphthenes, vol%		14.3	28.6	21.4	32.9	28.2	30.2	30.2		
Aromatics, vol%		0.0	13.7	16.5	20.3	28.3	40.8	38.4		
Thiophenes, vol%										
Molecular Weight	320	102	116	150	177	228	308	456	1080	525
Gross Heating Value, MM BTU/bbl	6.01	4.83	5.32	5.50	5.66	5.83	6.07	6.22	6.44	6.30
Gross Heating Value, kcal/kg	10530	11610	11230	11140	10990	10750	10470	10280	9740	10080
Gross Heating Value, MJ/kg	44.1	48.6	47.0	46.6	46.0	45.0	43.8	43.0	40.8	42.2
Heptane Asphaltenes, wt%	6.1								18.5	9.4
Micro Carbon Residue, wt%	11.3								34.2	17.3
Ramsbottom Carbon, wt%	10.5								32.0	16.2
Vanadium, ppm	47								144	73
Nickel, ppm	22								67	34
Iron, ppm	4								12	6

Complete crude oil assay of Ratawi crude oil

BRENT - SUMMARY OF MAJOR CUTS

	Whole Crude	Light Naphtha	Medium Naphtha	Heavy Naphtha	Kero	Atm Gas Oil	Light VGO	Heavy VGO	Vacuum Resid	Atm Resid
TBP Temp At Start, °C	Start	10	80	150	200	260	340	450	570	340
TBP Temp At End, °C	End	80	150	200	260	340	450	570	End	End
TBP Temp At Start, °F	Start	55	175	300	400	500	650	850	1050	650
TBP Temp At End, °F	End	175	300	400	500	650	850	1050	End	End
Yield at Start, vol%		3.4	11.3	27.1	37.1	47.1	61.8	78.3	89.8	61.8
Yield at End, vol%		11.3	27.1	37.1	47.1	61.8	78.3	89.8	100.0	100.0
Yield of Cut (wt% of Crude)		6.3	14.4	9.4	9.9	15.1	17.6	12.7	12.3	42.6
Yield of Cut (vol% of Crude)		8.0	15.8	10.0	10.0	14.8	16.5	11.5	10.2	38.2
Gravity, °API	38.5	83.2	54.4	48.2	40.9	35.1	27.9	22.1	10.3	21.1
Specific Gravity	0.8311	0.6591	0.7611	0.7874	0.8210	0.8494	0.8877	0.9212	0.9982	0.9273
Sulfur, wt%	0.43	0.00	0.00	0.01	0.04	0.25	0.57	0.82	1.44	0.90
Mercaptan Sulfur, ppm		3	5	4	4	3	3			
Nitrogen, ppm	1040			0	1	54	736	1910	5376	2423
Hydrogen, wt%	13.3	16.3	14.2	13.9	13.6	13.3	12.7	12.5	10.8	12.1
Viscosity @ 40 °C (104 °F), cSt	3.55			0.954	1.60	4.08	21.2	180	2.17E+05	189
Viscosity @ 50 °C (122 °F), cSt	2.94			0.853	1.37	3.24	14.6	102	51400	107
Viscosity @ 100 °C (212 °F), cSt	1.45		0.382	0.552	0.755	1.39	3.97	15.2	731	16.3
Viscosity @ 135 °C (275 °F), cSt	1.03			0.444	0.565	0.938	2.23	6.79	150	7.31
Freeze Point, °C			-100.000	-68.000	-42.000	-8.000	33.0	52.0		
Freeze Point, °F			-148	-90	-43	17	91	126		
Pour Point, °C	2		-114	-78	-49	-14	29	49	56	33
Pour Point, °F	35		-174	-109	-56	7	85	120	132	92
Smoke Point, mm (ASTM)				28	22	18	15	13		
Aniline Point, °C				53	61	71	83	93		
Aniline Point, °F				127	142	159	182	200		
Total Acid Number, mg KOH/g	0.05			0.0	0.0	0.0	0.0	0.1		
Cetane Index, ASTM D976				37	47	52				
Diesel Index				61	58	56	51	44		
Characterization Factor (K Factor)	12.1	12.8	11.7	11.8	11.8	11.9	12.0	12.1	11.8	11.9
Research Octane Number, Clear		65.2	56.8	43.3						
Motor Octane Number, Clear		63.8	54.7							
Paraffins, vol%		87.5	46.1	42.8	38.5	33.9	26.7	25.3		
Naphthenes, vol%		12.5	40.4	37.2	39.9	41.2	43.1	43.2		
Aromatics, vol%		0.0	13.5	19.9	21.5	24.9	30.2	31.6		
Thiophenes, vol%										
Molecular Weight	209	102	113	143	176	225	317	468	880	418
Gross Heating Value, MM BTU/bbl	5.76	4.82	5.37	5.52	5.70	5.85	6.03	6.18	6.47	6.20
Gross Heating Value, kcal/kg	10990	11580	11210	11140	11030	10940	10760	10660	10290	10620
Gross Heating Value, MJ/kg	46.0	48.5	46.9	46.6	46.2	45.8	45.0	44.6	43.1	44.5
Heptane Asphaltenes, wt%	0.4								3.1	0.9
Micro Carbon Residue, wt%	1.9								15.6	4.5
Ramsbottom Carbon, wt%	1.8								14.8	4.3
Vanadium, ppm	7								58	17
Nickel, ppm	1								11	3
Iron, ppm										

Complete crude oil assay of Brent crude

Appendix B (Crude oil cost)

The cost of the crudes were obtained from EIA

Week Of	Mon	Tue	Wed	Thu	Fri
2011 Feb-14 to Feb-18	103.12	102.48	102.78	103.45	102.20
2011 Feb-21 to Feb-25		106.82	109.77	113.91	111.47
2011 Feb-28 to Mar- 4	112.27	113.34	116.89	114.42	115.71
2011 Mar- 7 to Mar-11	116.58	112.32	115.19	114.07	114.07
2011 Mar-14 to Mar-18	112.95	111.11	110.96	114.18	114.13
2011 Mar-21 to Mar-25	114.92	115.63	115.65	115.41	115.45
2011 Mar-28 to Apr- 1	115.95	115.58	115.35	116.94	118.63
2011 Apr- 4 to Apr- 8	120.07	122.87	123.01	122.90	126.30
2011 Apr-11 to Apr-15	126.46	121.33	122.70	122.74	124.63
2011 Apr-18 to Apr-22	121.69	121.35	124.26	123.64	
2011 Apr-25 to Apr-29		124.55	124.94	126.59	
2011 May- 2 to May- 6	126.64	124.01	121.55	111.93	113.69
2011 May- 9 to May-13	113.21	117.82	115.66	112.87	113.08
2011 May-16 to May-20	113.72	109.39	112.54	113.20	111.25
2011 May-23 to May-27	110.13	112.52	114.47	115.06	114.85
2011 May-30 to Jun- 3		117.18	116.15	114.30	115.09
2011 Jun- 6 to Jun-10	115.40	116.14	118.43	119.95	118.71
2011 Jun-13 to Jun-17	120.49	120.35	114.67	114.69	113.74
2011 Jun-20 to Jun-24	112.21	112.02	113.59	108.27	104.79
2011 Jun-27 to Jul- 1	104.57	107.57	111.49	111.71	109.82
2011 Jul- 4 to Jul- 8		113.21	113.55	117.40	117.40
2011 Jul-11 to Jul-15	117.35	117.36	118.46	117.38	118.06
2011 Jul-18 to Jul-22	117.05	118.18	118.52	118.25	118.99
2011 Jul-25 to Jul-29	118.27	118.14	117.99	118.16	115.93

Table B- 1 Week Brent FOB in Dollars per Barrel (EIA, 2011)

	Week 1		Week 2		Week 3		Week 4		Week 5	
Year-Month	End Date	Value	End Date	Value	End Date	Value	End Date	Value	End Date	Value
2008-Dec	12/05	35.70	12/12	28.32	12/19	29.89	12/26	21.03		
2009-Jan	01/02	23.58	01/09	30.72	01/16	32.92	01/23	31.61	01/30	36.94
2009-Feb	02/06	33.56	02/13	35.63	02/20	31.55	02/27	34.70		
2009-Mar	03/06	34.97	03/13	40.48	03/20	43.45	03/27	48.28		
2009-Apr	04/03	46.16	04/10	45.72	04/17	45.46	04/24	43.09		
2009-May	05/01	44.60	05/08	48.39	05/15	52.27	05/22	53.22	05/29	56.91
2009-Jun	06/05	59.93	06/12	61.27	06/19	65.52	06/26	63.94		
2009-Jul	07/03	64.60	07/10	58.03	07/17	52.51	07/24	55.39	07/31	59.40
2009-Aug	08/07	60.86	08/14	64.97	08/21	63.38	08/28	66.15		
2009-Sep	09/04	57.15	09/11	65.40	09/18	66.64	09/25	65.82		
2009-Oct	10/02	61.90	10/09	64.21	10/16	65.33	10/23	70.92	10/30	73.25
2009-Nov	11/06	71.05	11/13	69.27	11/20	68.12	11/27	66.97		
2009-Dec	12/04	66.05	12/11	66.55	12/18	61.36	12/25	63.40		
2010-Jan	01/01	68.53	01/08	74.27	01/15	75.99	01/22	72.08	01/29	70.30
2010-Feb	02/05	66.68	02/12	68.35	02/19	70.49	02/26	74.02		
2010-Mar	03/05	73.79	03/12	74.99	03/19	75.65	03/26	74.88		
2010-Apr	04/02	76.11	04/09	79.69	04/16	78.74	04/23	75.48	04/30	75.26
2010-May	05/07	75.01	05/14	65.07	05/21	59.93	05/28	56.34		
2010-Jun	06/04	57.73	06/11	63.10	06/18	66.31	06/25	67.61		
2010-Jul	07/02	69.65	07/09	73.15	07/16	64.35	07/23	64.83	07/30	66.84
2010-Aug	08/06	68.65	08/13	71.16	08/20	67.28	08/27	62.92		
2010-Sep	09/03	63.14	09/10	63.05	09/17	63.36	09/24	56.28		
2010-Oct	10/01	57.41	10/08	61.24	10/15	61.46	10/22	60.28	10/29	60.47
2010-Nov	11/05	64.58	11/12	76.80	11/19	74.55	11/26	71.98		
2010-Dec	12/03	74.68	12/10	78.93	12/17	78.53	12/24	77.80	12/31	80.67
2011-Jan	01/07	78.71	01/14	74.96	01/21	76.83	01/28	73.90		
2011-Feb	02/04	75.38	02/11	73.15	02/18	65.00	02/25	67.47		
2011-Mar	03/04	78.96	03/11	87.51	03/18	85.56	03/25	85.88		
2011-Apr	04/01	90.27	04/08	93.36	04/15	99.89	04/22	98.01	04/29	100.21
2011-May	05/06	101.54	05/13	95.53	05/20	90.81	05/27	89.44		
2011-Jun	06/03	89.93	06/10	90.20	06/17	87.23	06/24	87.23		
2011-Jul	07/01	79.99	07/08	87.40	07/15	86.85	07/22	88.58	07/29	88.58

Table B- 2 Week Ratawi crude oil FOB in Dollars per Barrel (EIA, 2011)

Appendix C (Charts used for Empirical correlations)

The charts in appendix C were used for empirical correlations for FCC yields. The Figure 1 was used to determine the conversion rate of the feed from FCC. The other charts were then used to calculate the composition of the intermediate products from the FCC unit. Figure 11 is an example of how the products from the FCC unit were calculated using 50/50 volumetric mixing ratio.

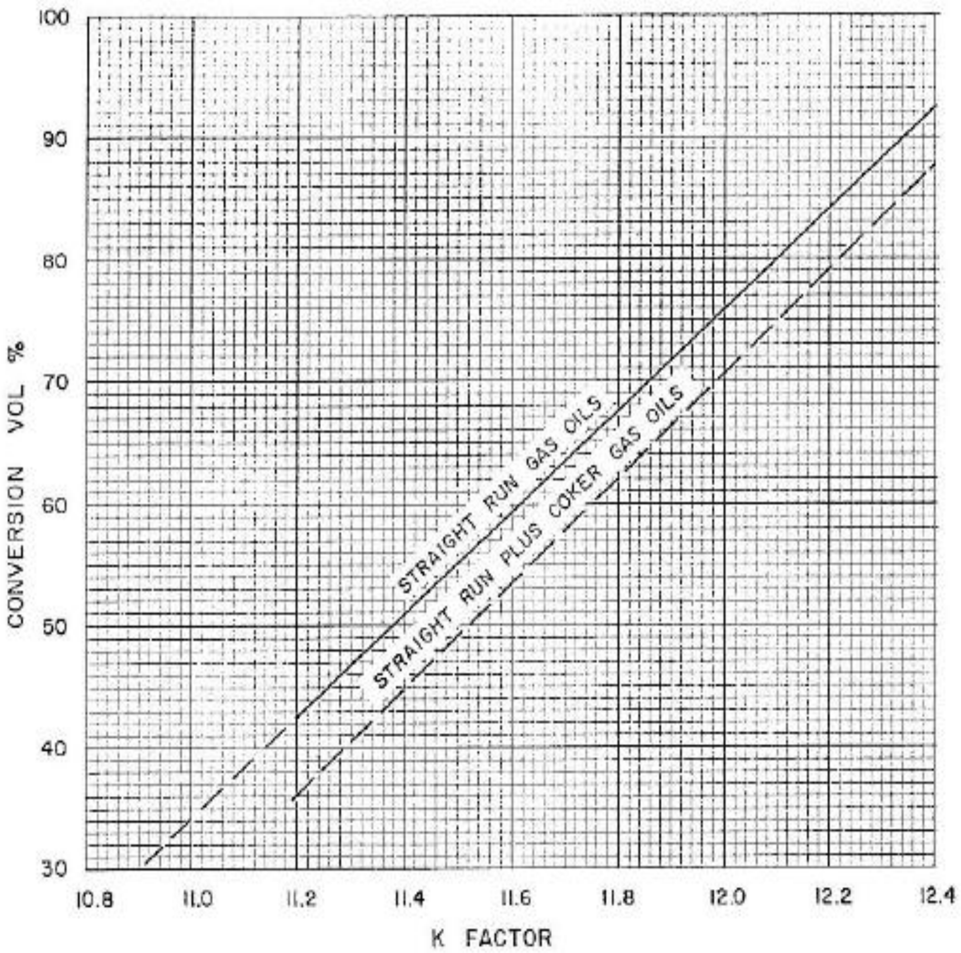


Figure 1Effect of feed composition on conversion at constant operating conditions

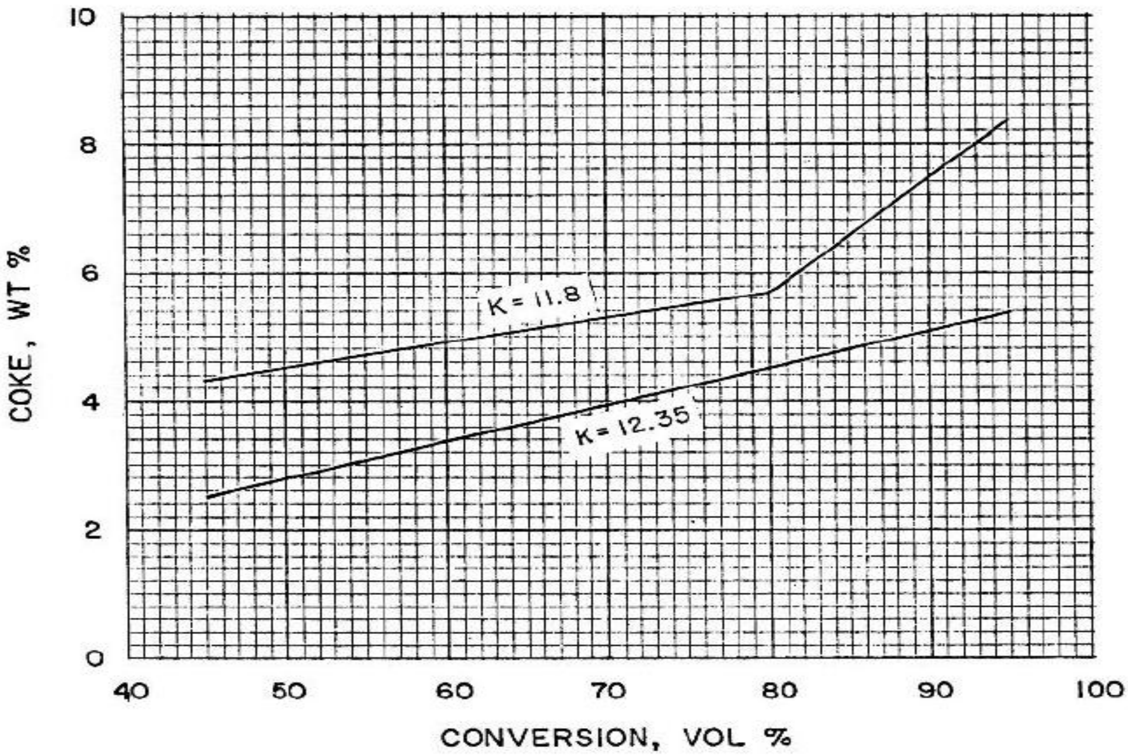


Figure 2 Catalytic Cracking yields, Zeolite catalyst (coke)

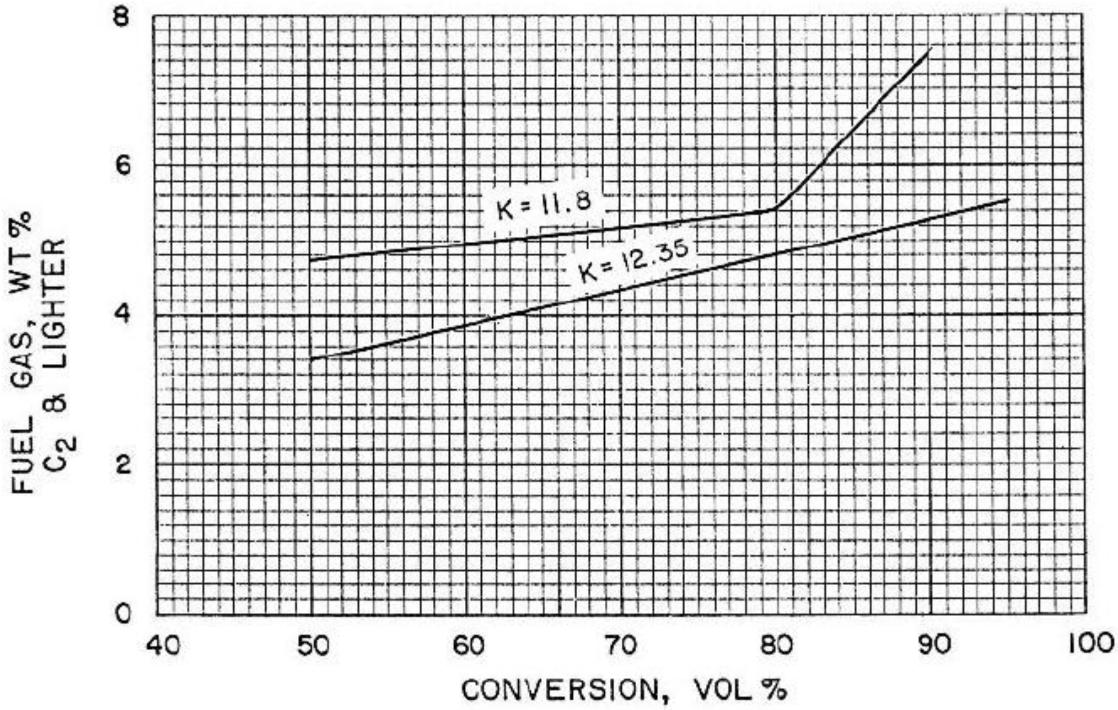


Figure 3 Catalytic Cracking yields, Zeolite catalyst (Fuel gas)

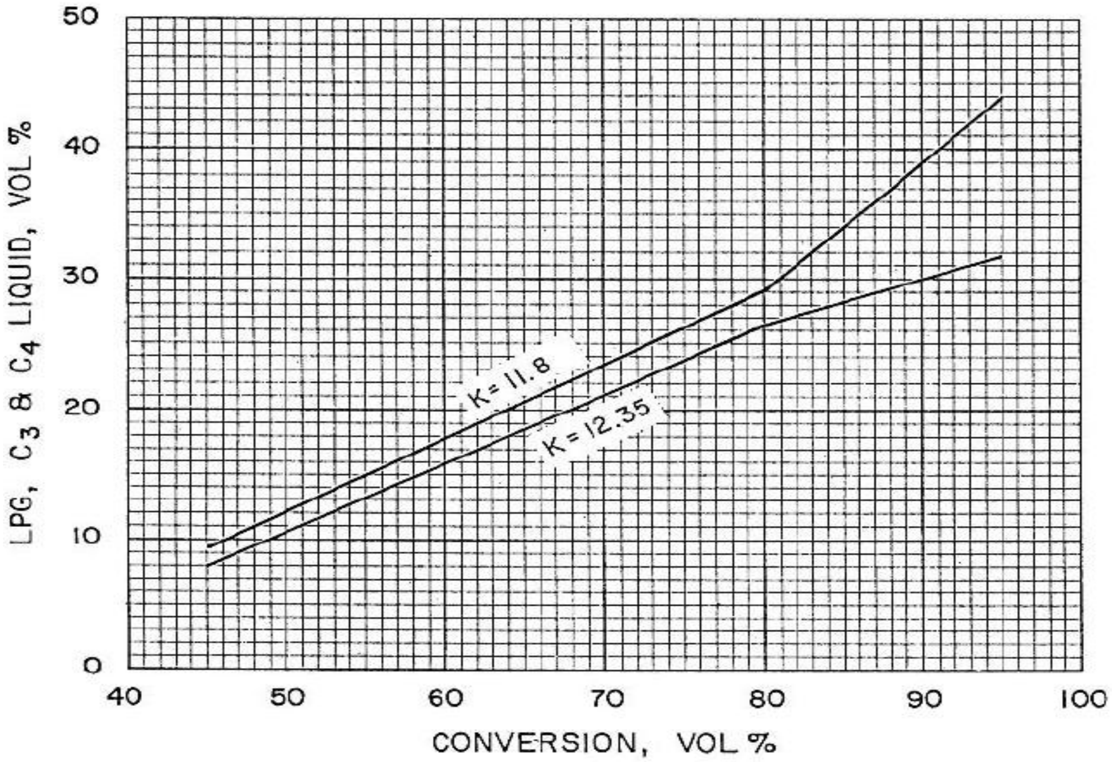


Figure 4 Catalytic Cracking yields, Zeolite catalyst (C3 and C4)

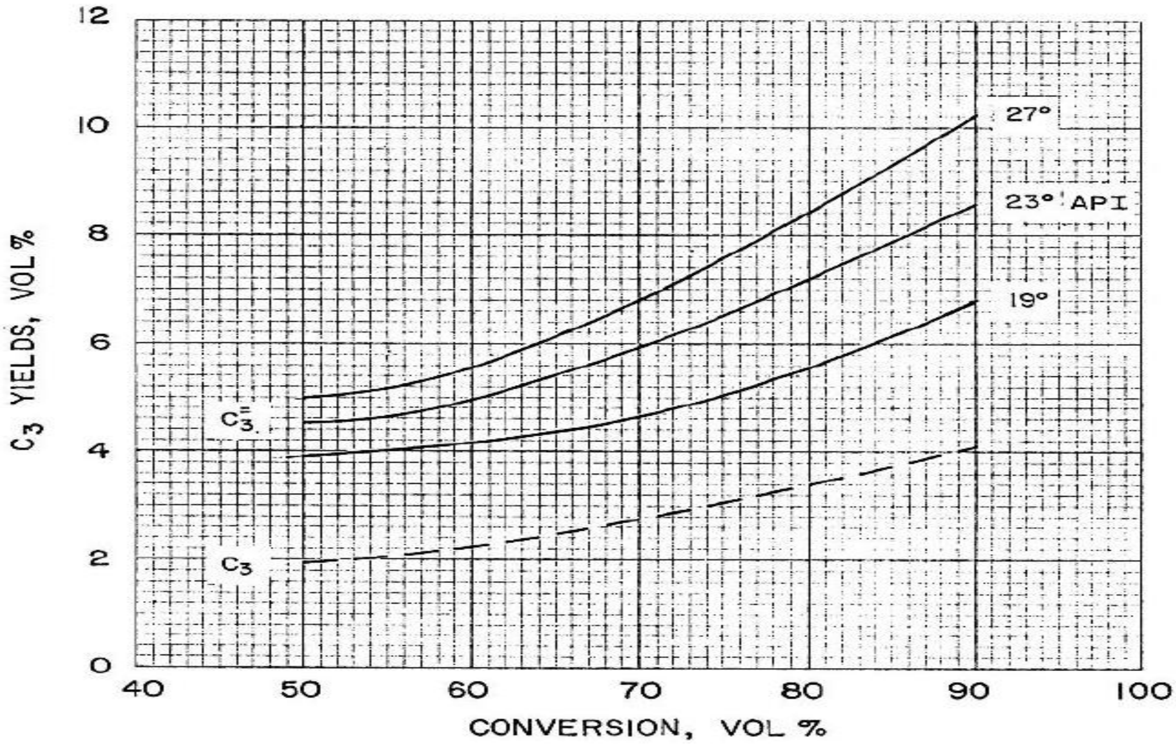


Figure 5 Catalytic Cracking yields, Zeolite catalyst (C3 ratios)

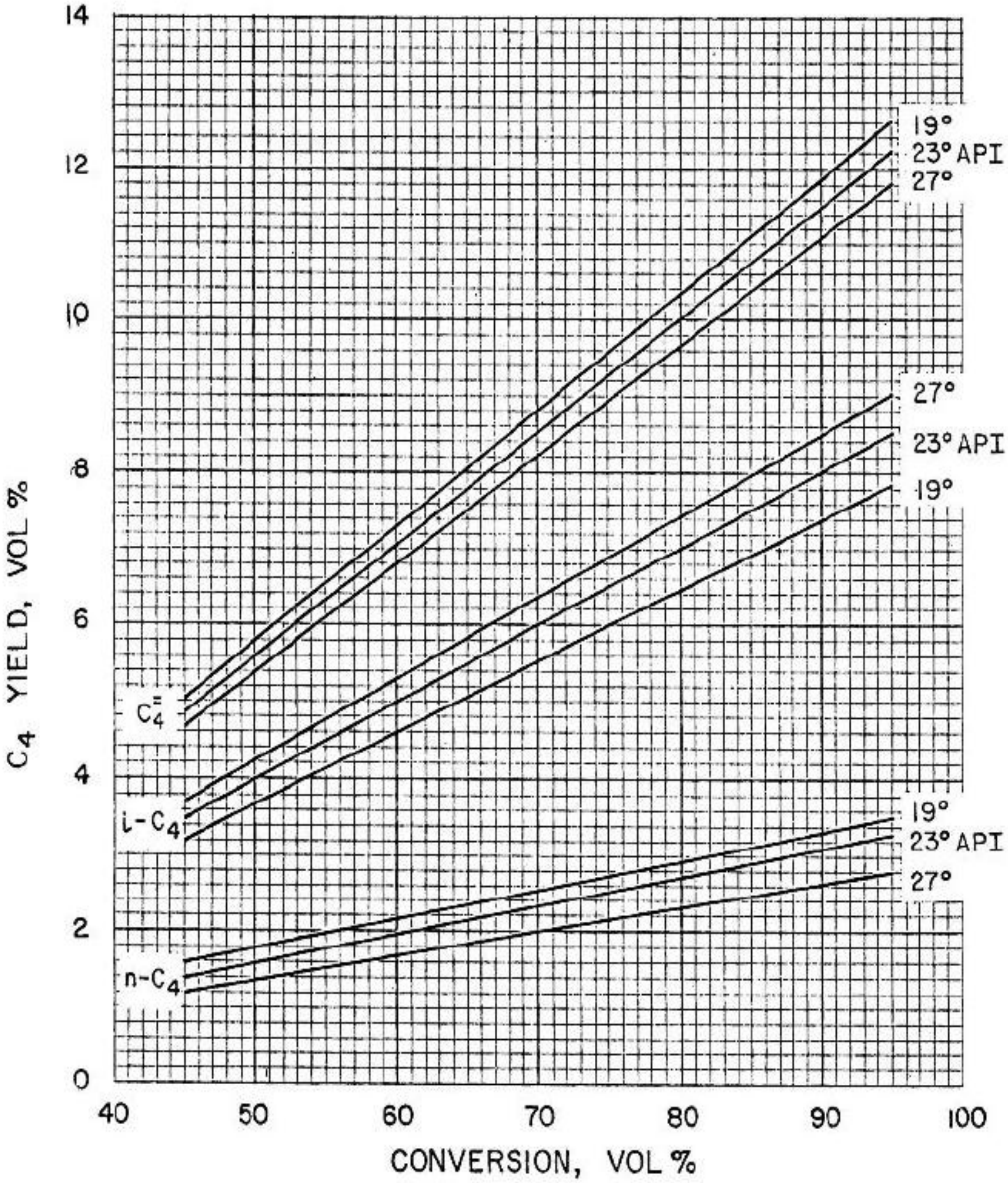


Figure 6 Catalytic Cracking yields, Zeolite catalyst (C4 ratios)

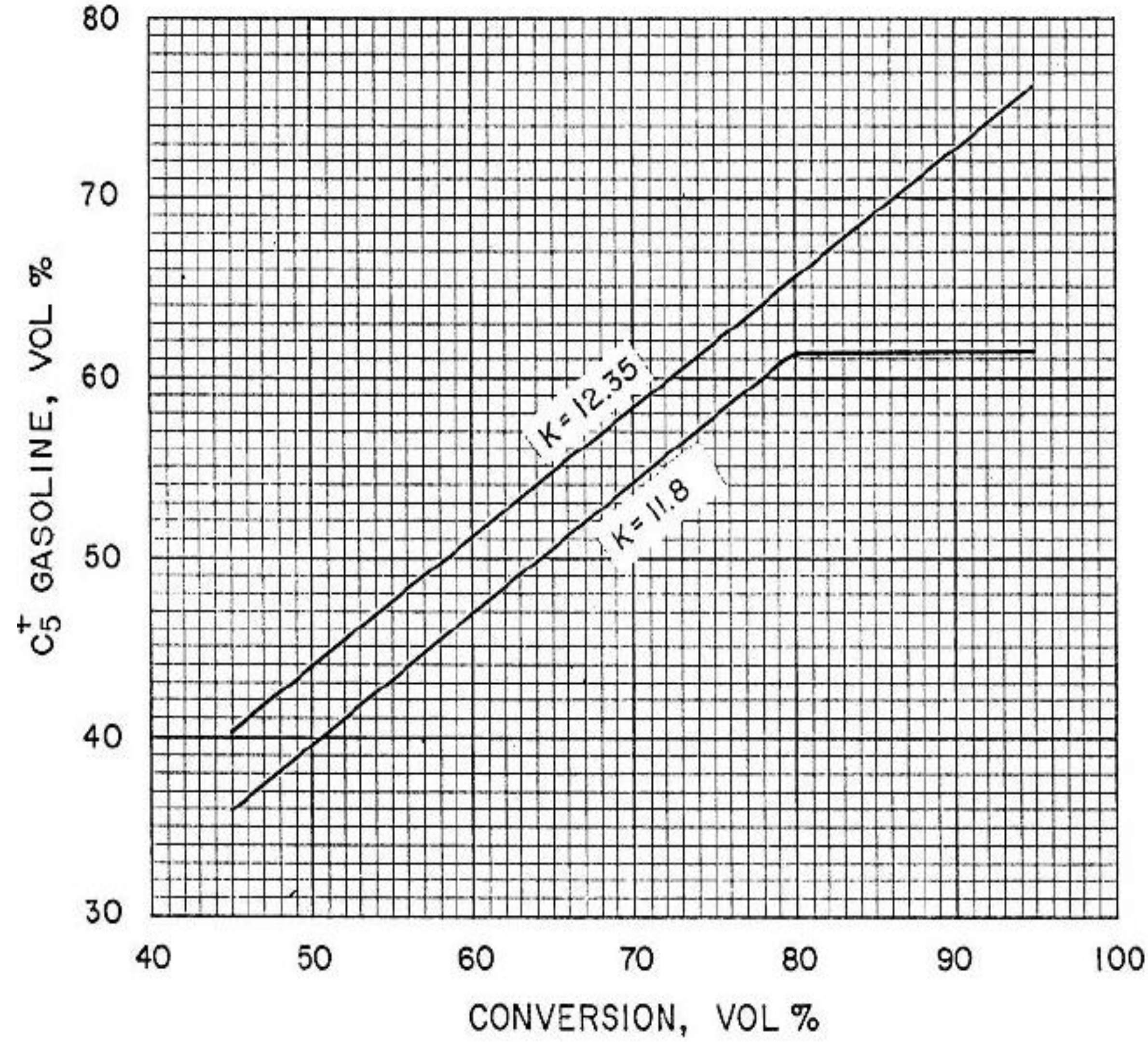


Figure 7 Catalytic Cracking yields, Zeolite catalyst (C5 + gasoline)

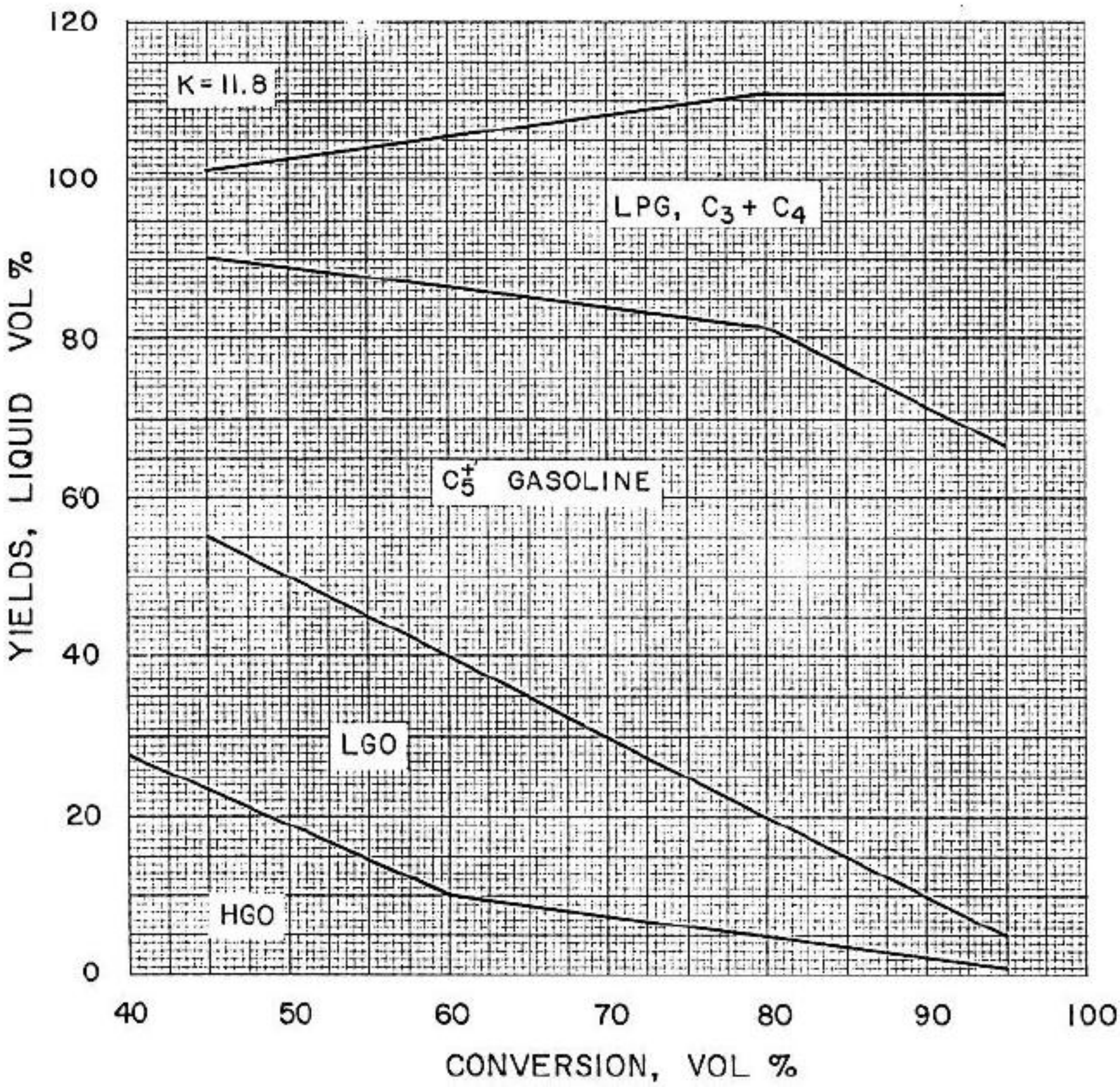


Figure 8 Catalytic Cracking yields, Zeolite catalyst (Heavy gas oil, feed K=11.8)

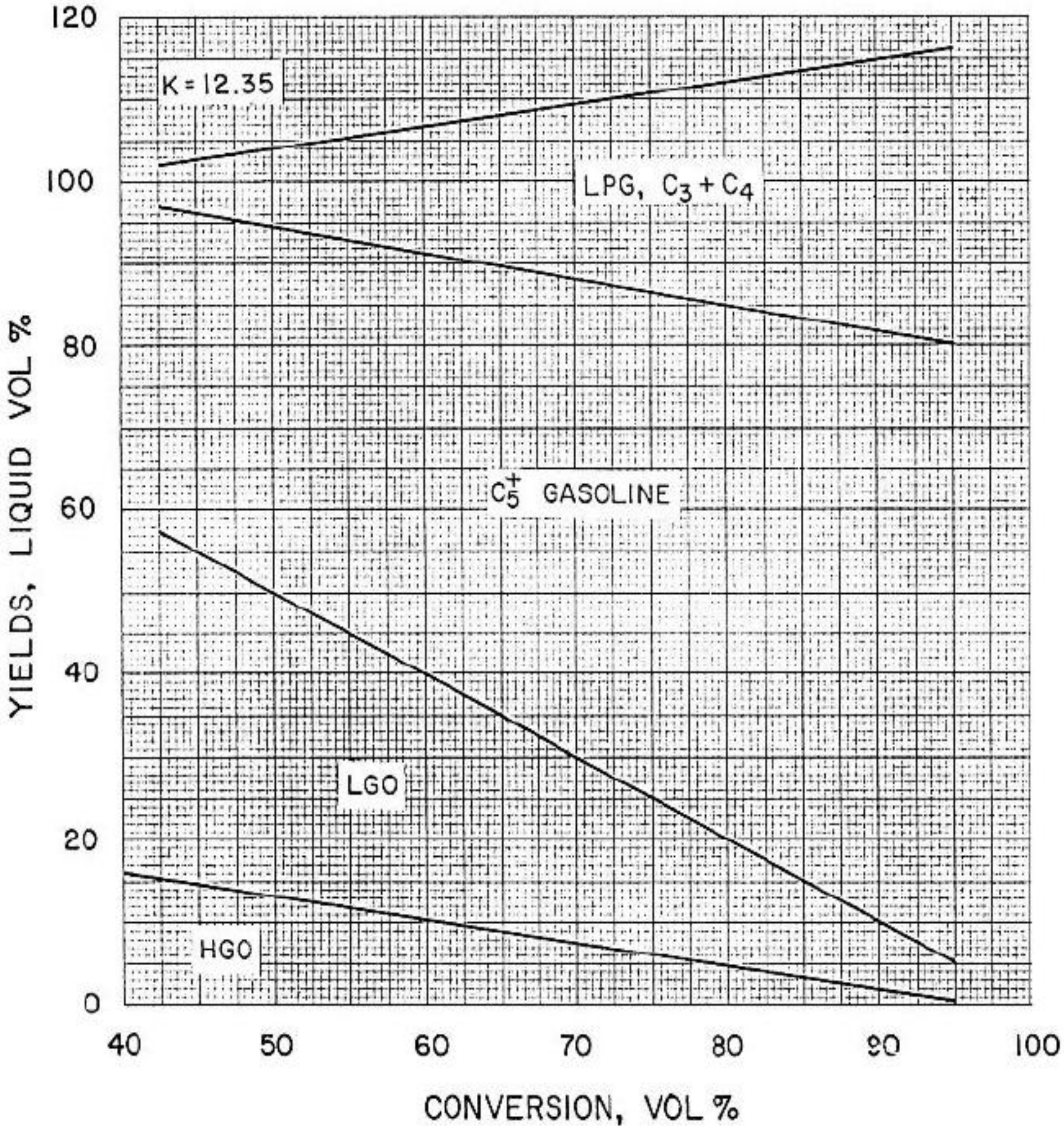


Figure 9 Catalytic Cracking yields, Zeolite catalyst (Heavy gas oil, feed K=12.35)

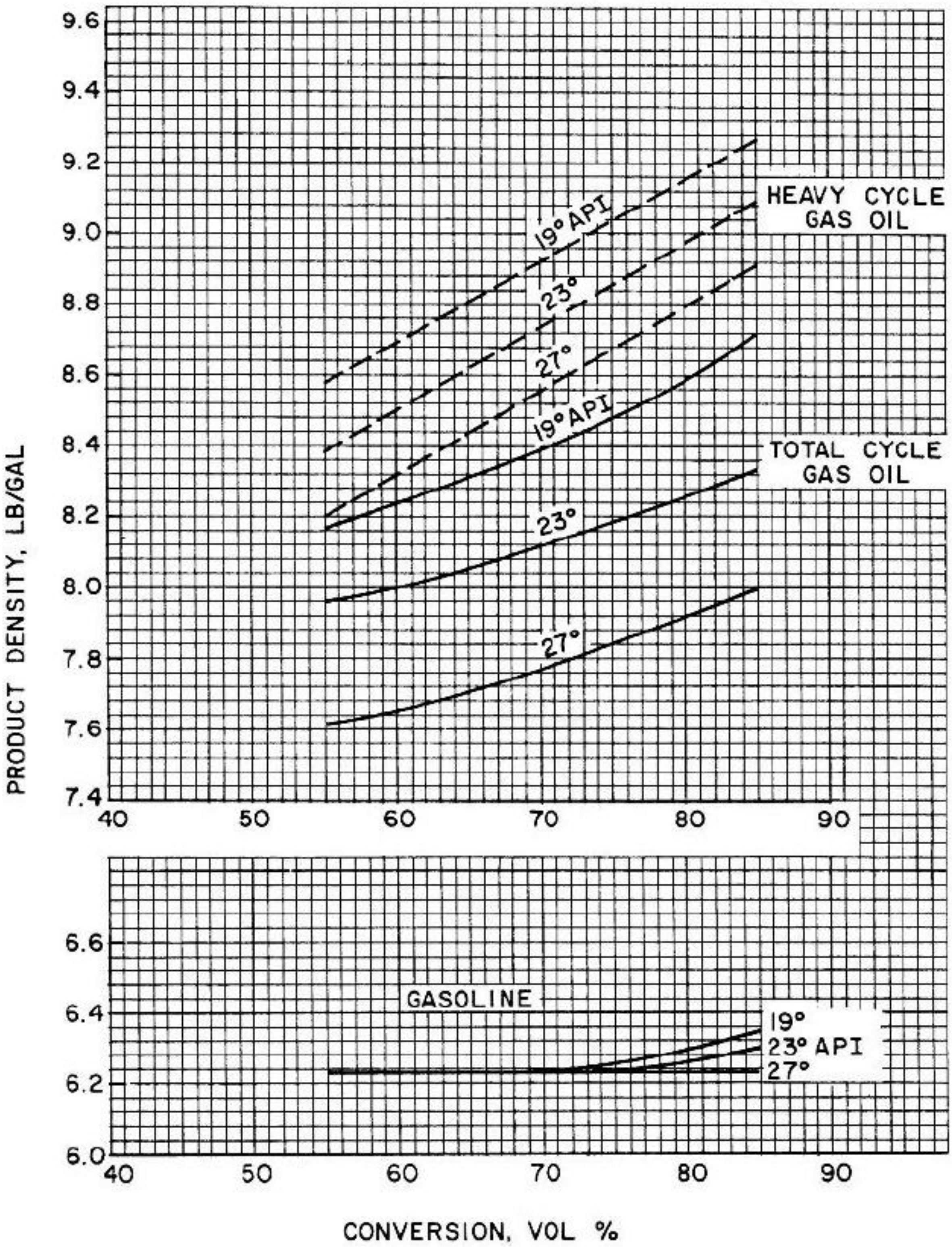
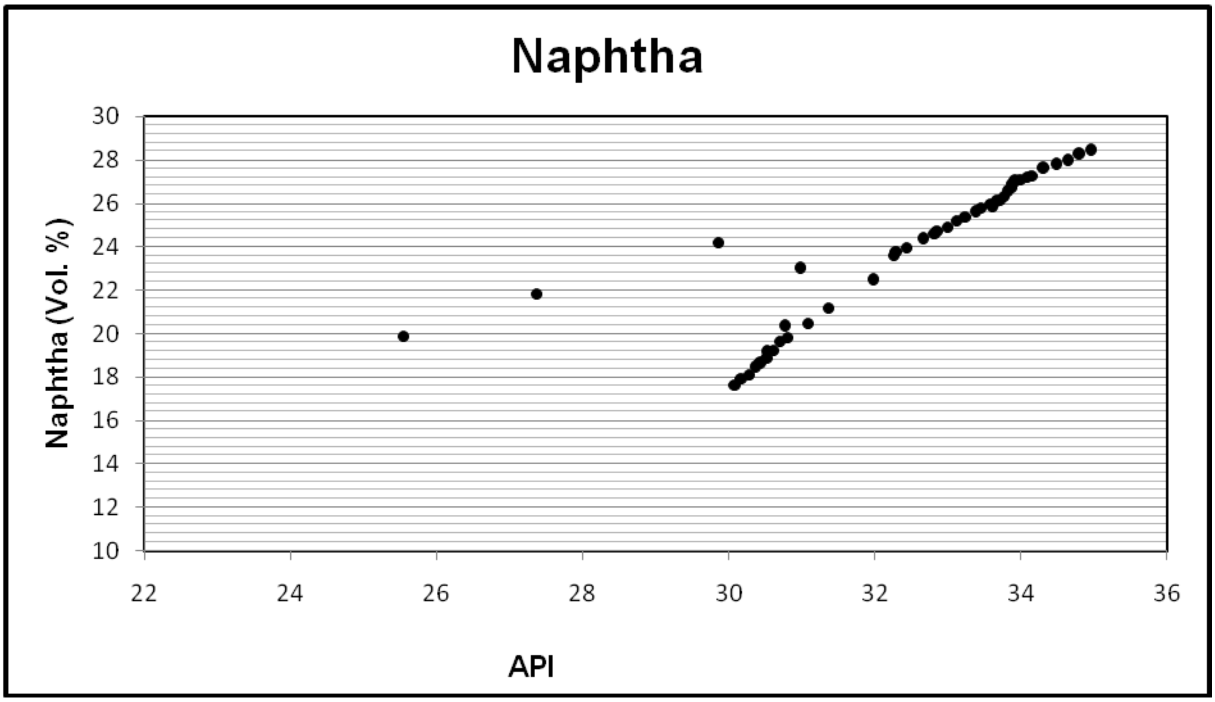


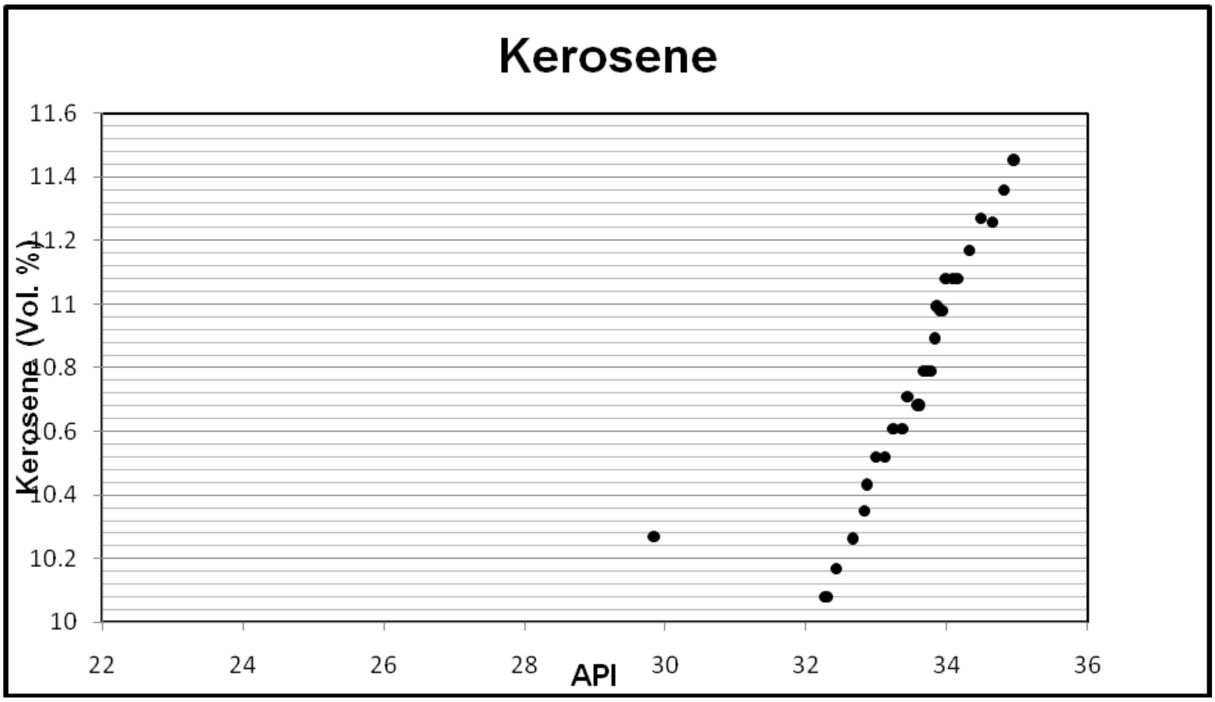
Figure 10 FCC product gravity Zeolite catalysts

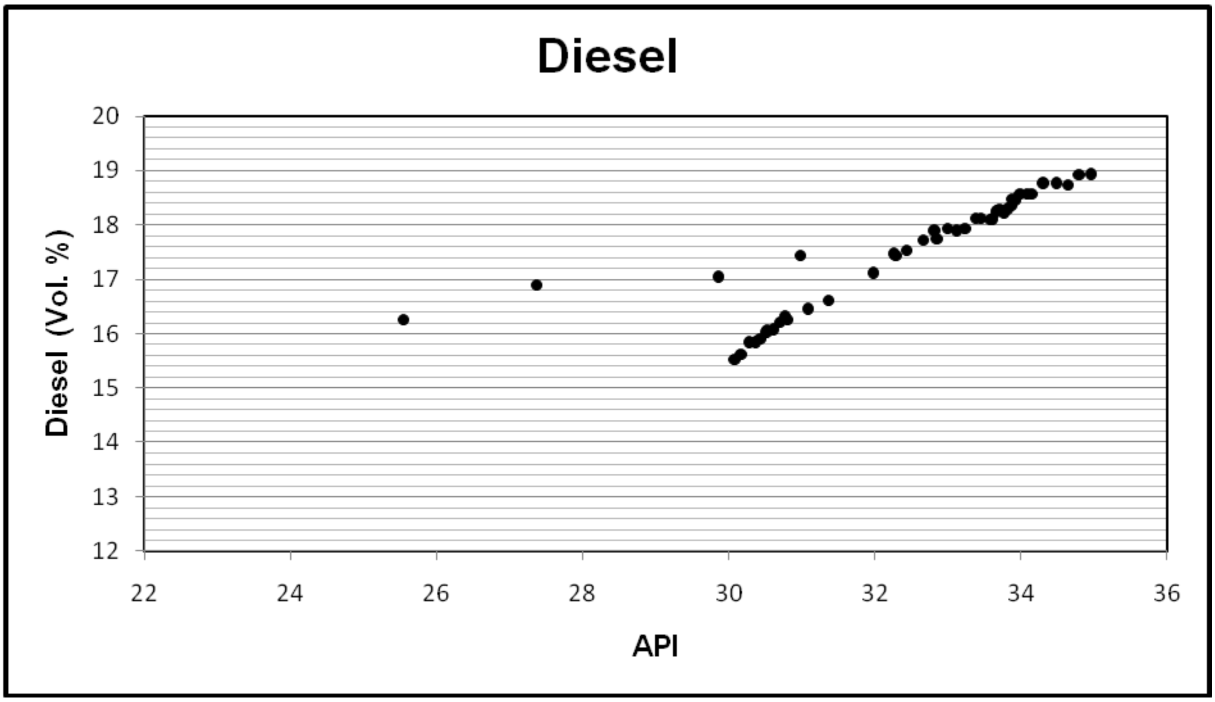
	50/50		Density	%vol. for 68% conversion	Wt %	wt (kg/hr)	Vol. (m^3/hr)
density to FCC	886.2	L.gas	413.3	-	5.1	5007.739	12.11647
volume	110.8	Lpg	553	0.22	13.72828	13479.93	24.376
mass	98190.96	Fcc gas	622.604	-	37.60138	36921.15	59.30118
		Coke	880	-	5.2	5105.93	5.802193
		TGO	850.095	0.4	38.37035	37676.21	44.32
					100	98190.96	145.9158

Figure 11Procedure for calculating the values for yields for FCC units

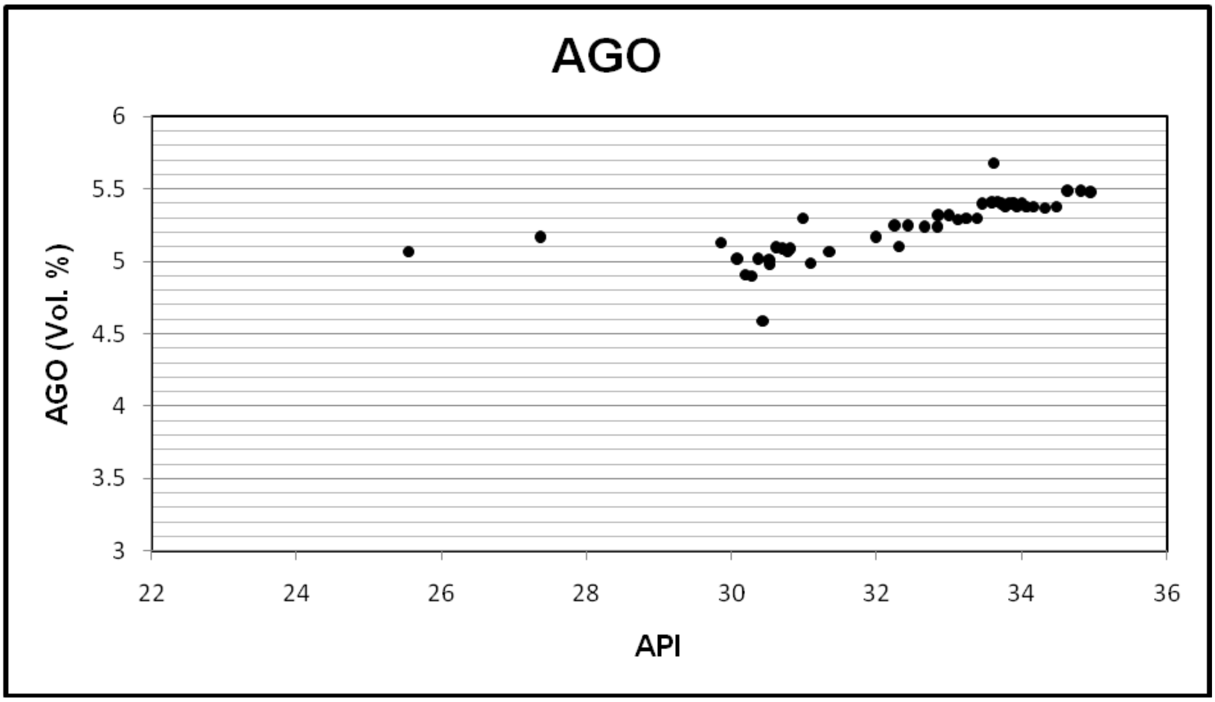
Appendix D (Graphs of Yields versus API)



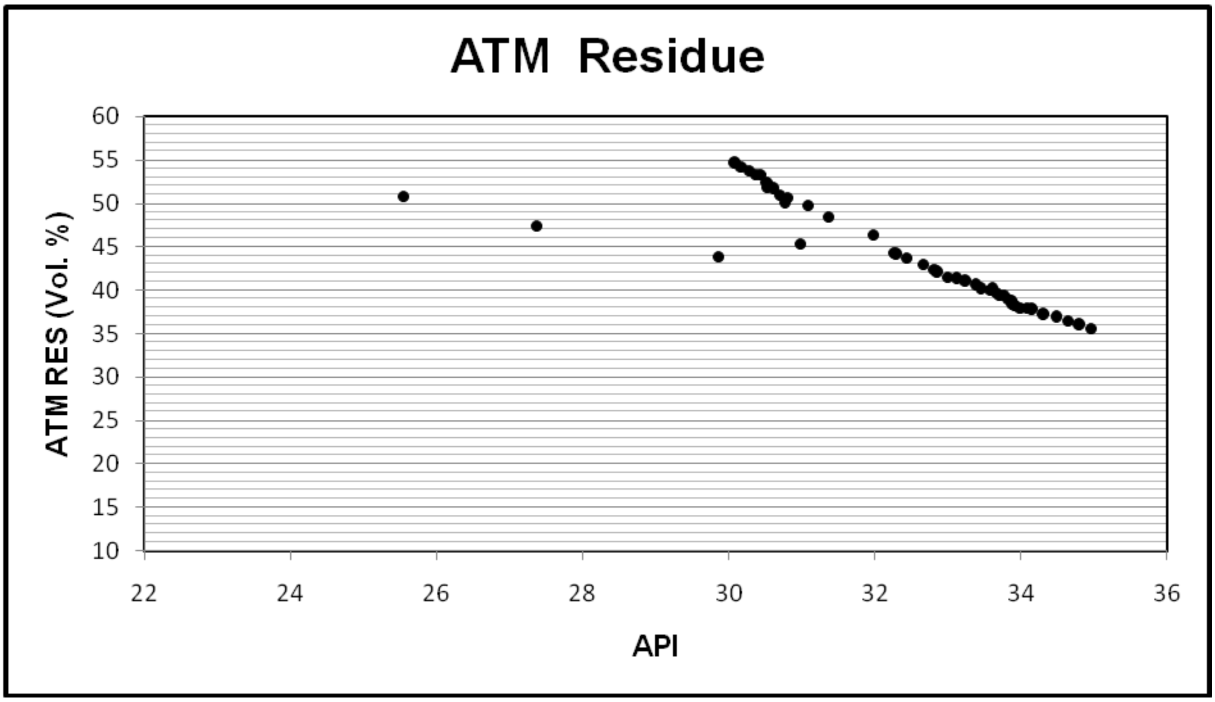


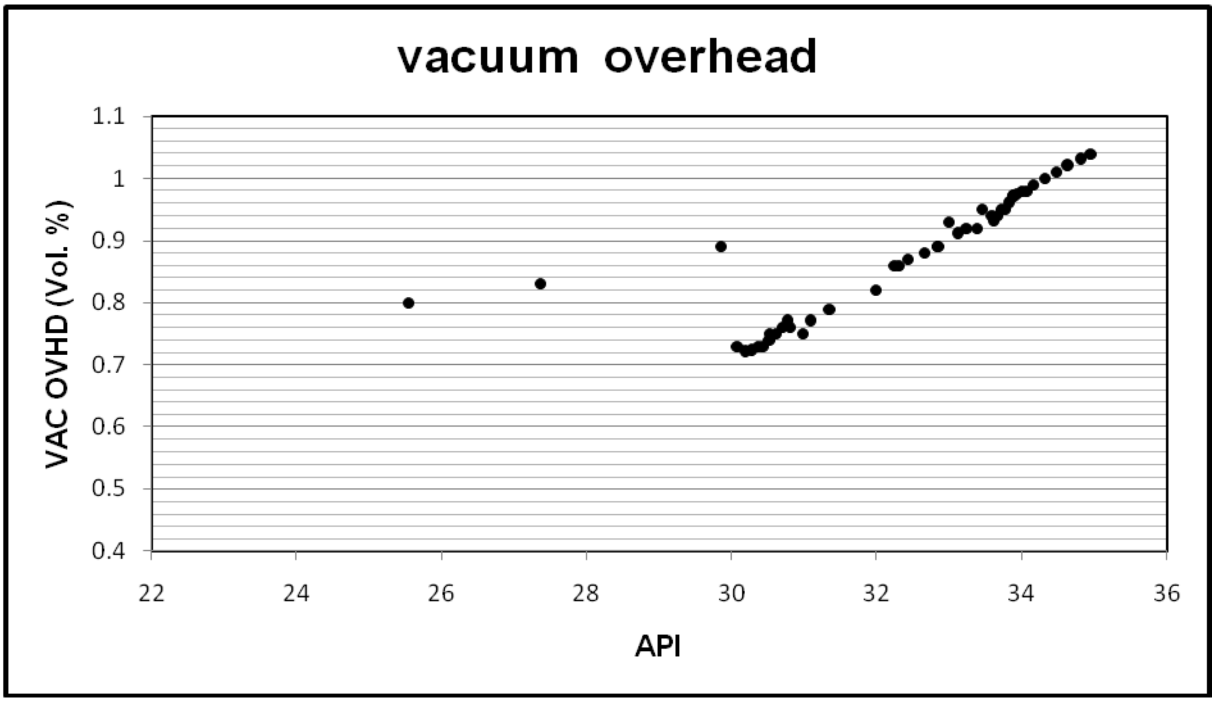


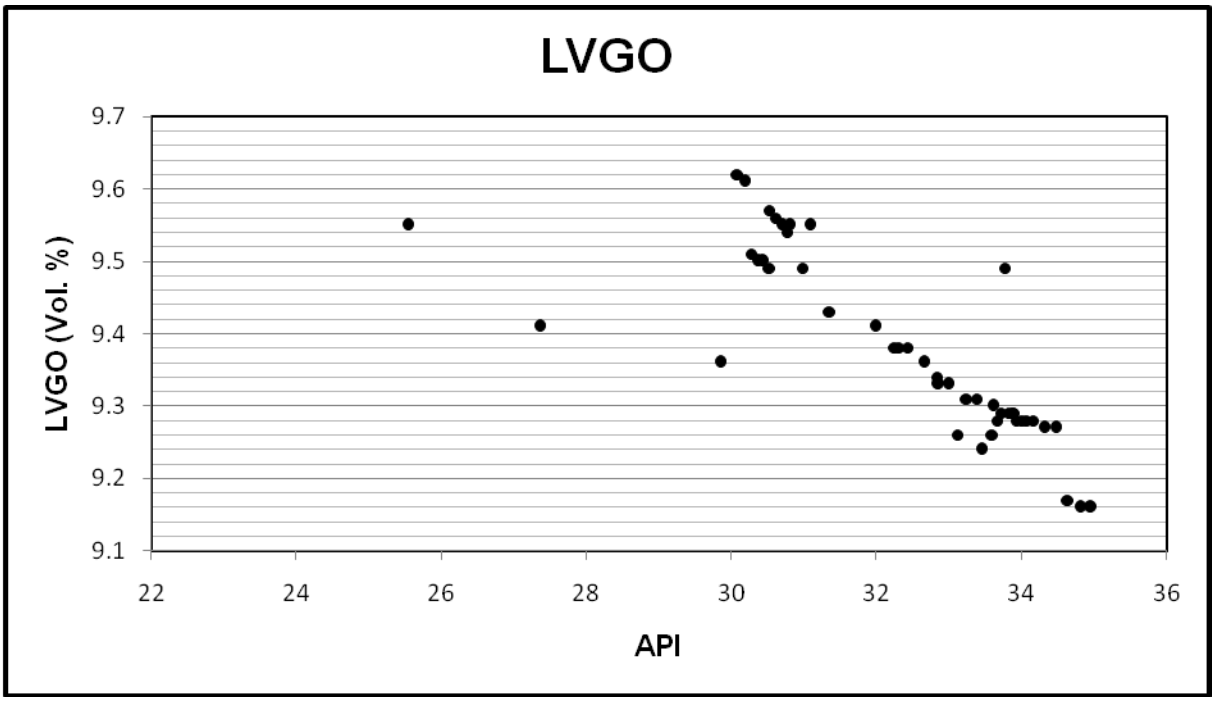
Diesel
20
19
18
17
16
15
14
13
12
Diesel (Vol. %)
22
24
26
28
30
32
34
36
API

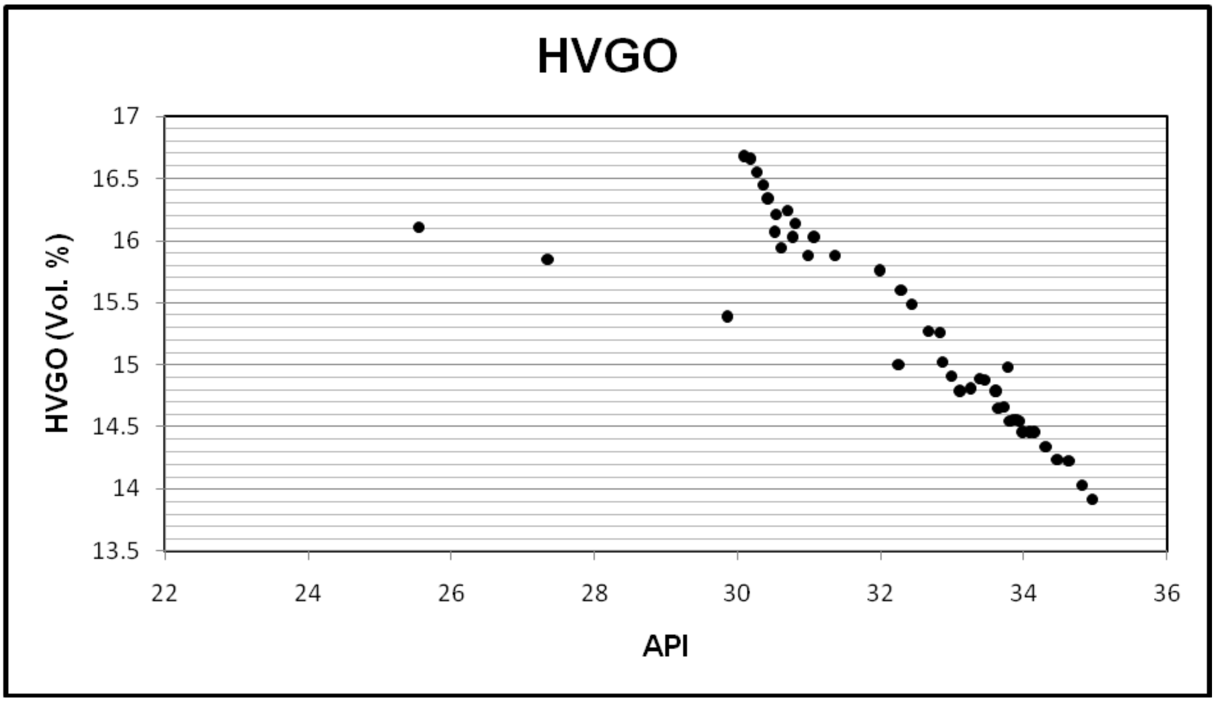


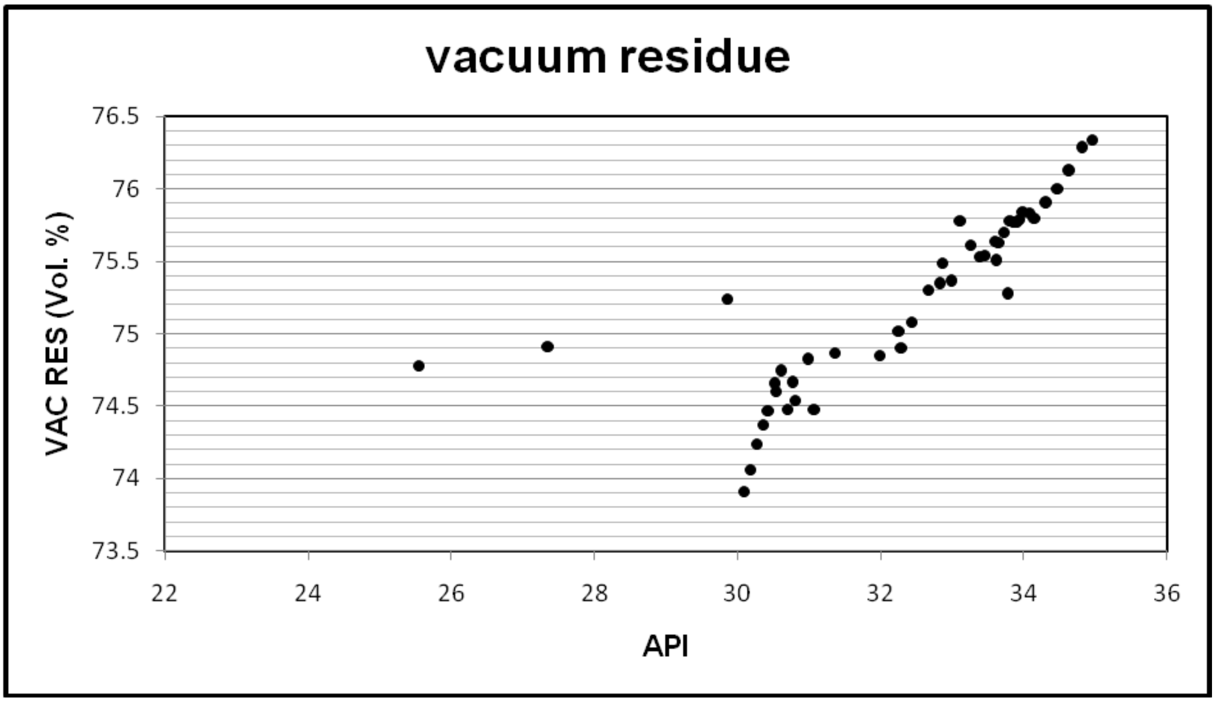
AGO
6
5.5
5
4.5
4
3.5
3
AGO (Vol. %)
22
24
26
28
30
32
34
36
API


ATM Residue
ATM RES (Vol. %)
60
55
50
45
40
35
30
25
20
15
10
22
24
26
28
30
32
34
36
API

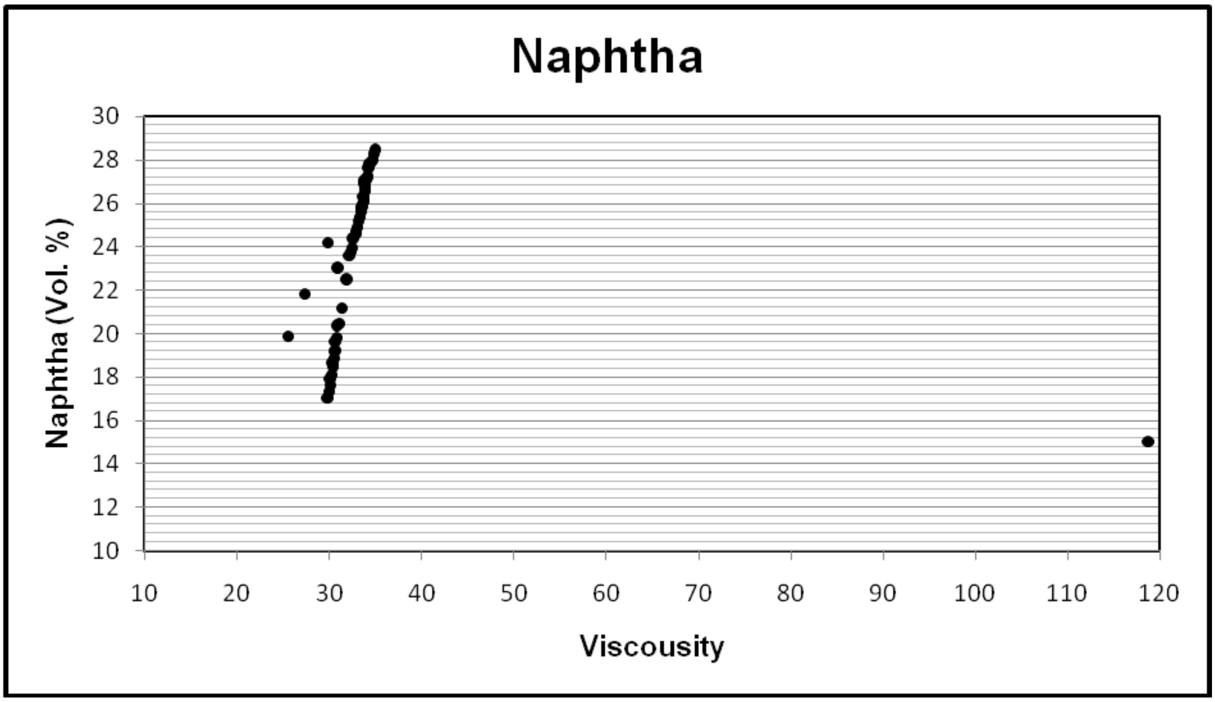

vacuum overhead
VAC OVHD (Vol. %)
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
22
24
26
28
30
32
34
36
API

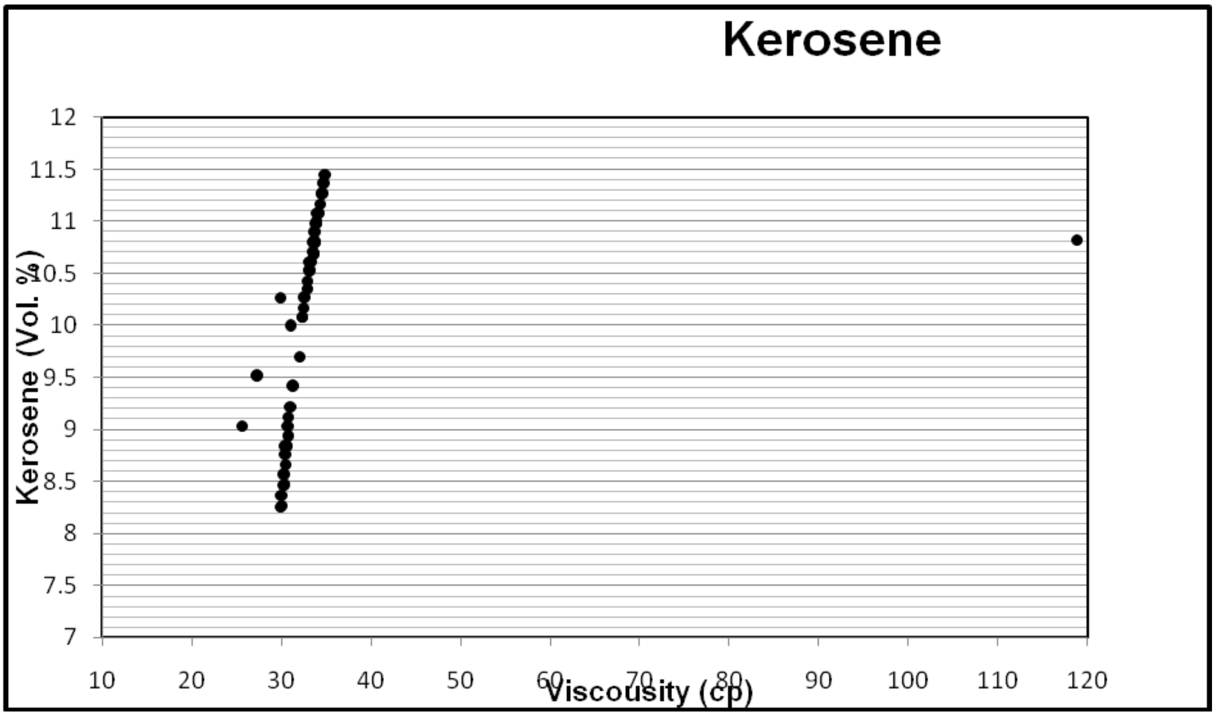

LVGO
9.7
9.6
9.5
9.4
9.3
9.2
9.1
LVGO (Vol. %)
22
24
26
28
30
32
34
36
API


HVGO
17
16.5
16
15.5
15
14.5
14
13.5
HVGO (Vol. %)
22
24
26
28
30
32
34
36
API

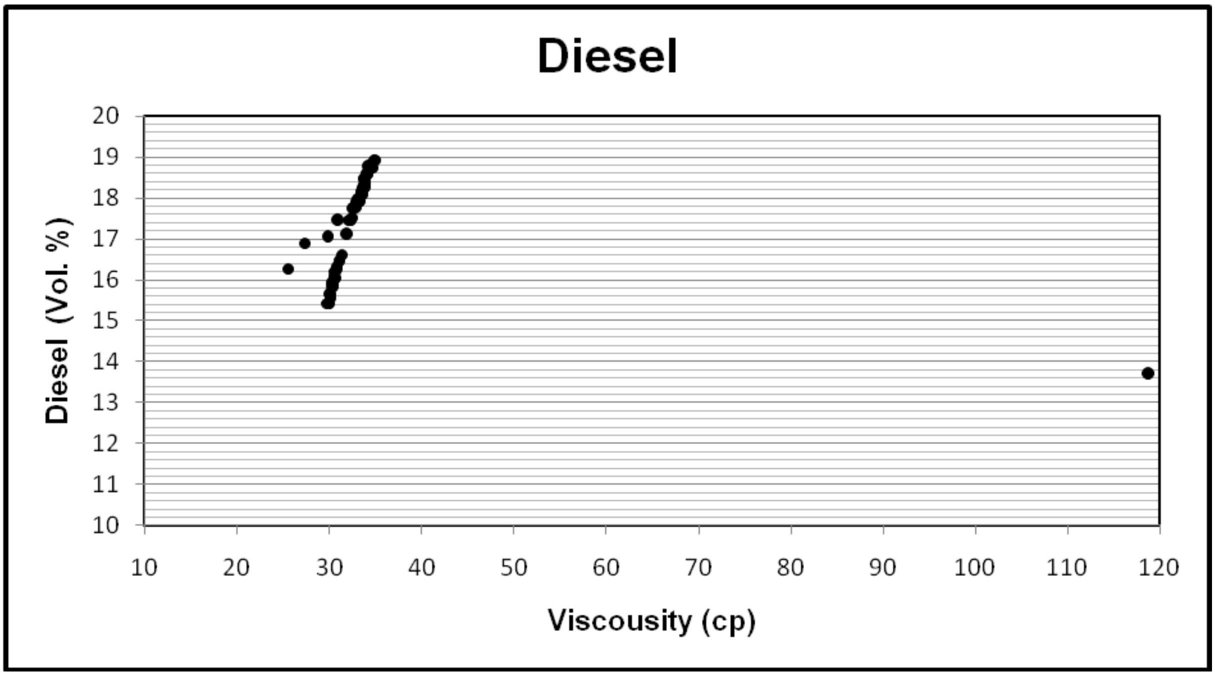

vacuum residue
VAC RES (Vol. %)
76.5
76
75.5
75
74.5
74
73.5
22
24
26
28
30
32
34
36
API

Appendix E (Graphs of Yields versus Viscosity)

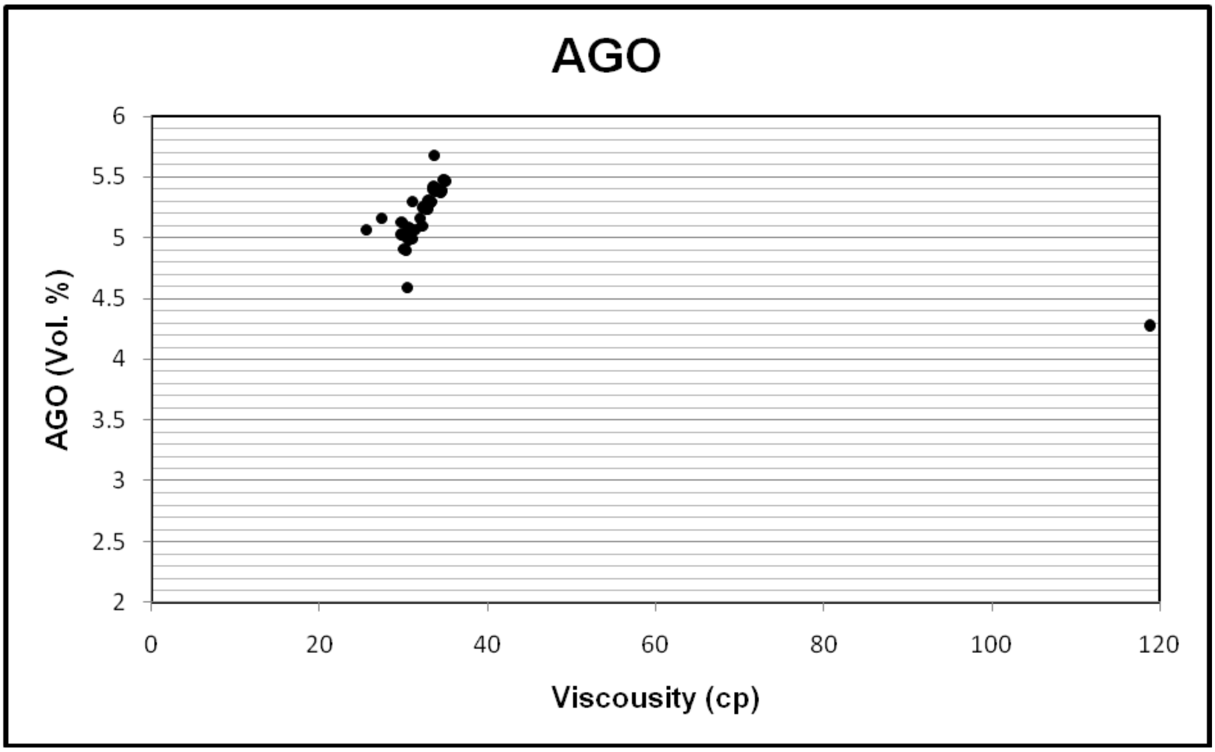




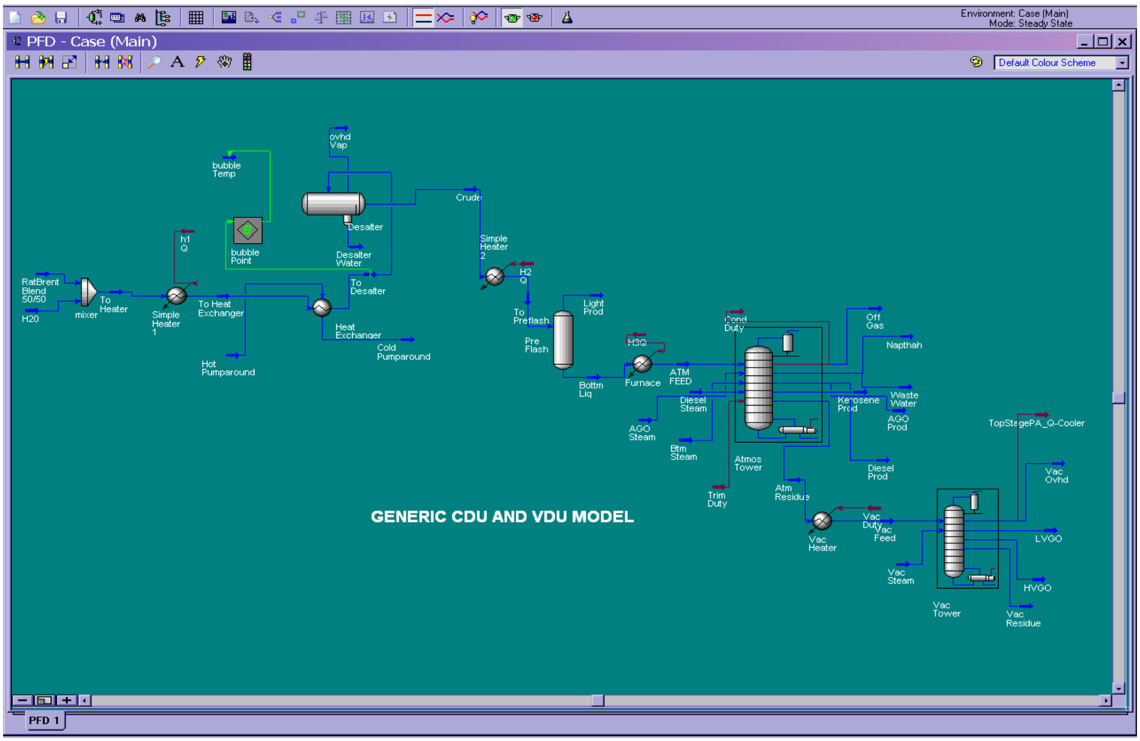
Kerosene
Kerosene (Vol. %)
Viscousity (cp)
12
11.5
11
10.5
10
9.5
9
8.5
8
7.5
7
10
20
30
40
50
60
70
80
90
100
110
120



Diesel
Diesel (Vol. %)
Viscousity (cp)
20
19
18
17
16
15
14
13
12
11
10
10
20
30
40
50
60
70
80
90
100
110
120



Appendix F (Process flow sheet)



Appendix G Conversion from ASTM to TBP (Li 2000) Polynomial Regression Method

A	Ci	Naphtha	Kerosene	Diesel	AGO	Atm Res
0	-89.99134827	-89.99134827	-89.99134827	-89.99134827	-89.99134827	-89.991348
1	2.74798583	875.783084	1227.52527	1739.749829	2016.746801	4215.41026
2	-0.01068849	-1085.626616	-2132.790807	-4284.113639	-5756.919155	-25151.684
3	3.17355E-05	1027.285315	2828.738145	8053.076598	12544.56345	114556.825
4	-4.87231E-08	-502.6474974	-1939.988166	-7827.526108	-14134.57718	-269796.75
5	3.72814E-11	122.5752578	663.0896673	3791.875467	7937.375688	316679.023
6	-1.11569E-14	-11.69058543	-88.64200972	-718.4189184	-1743.272203	-145377.11
	SUM	335.6876096	467.9407512	664.6518797	773.9260539	-4964.2767

Appendix H (Details of Rigorous runs in AspenHYSYS)

RAT	88.58														
BRENT	115.93														
%RAT	0	2	4	6	8	10	12	14	16	18	20	22	24	25	26
% BRENT	100	98	96	94	92	90	88	86	84	82	80	78	76	75	74
SCENARIOS	0_100	2_98	4_96	6_94	8_92	10_90	12_88	14_86	16_84	18_82	20_80	22_78	24_76	25_75	26_74
NAPHTHA	25.29	28.42	28.24	27.95	27.77	27.58	27.28	27.1	26.91	26.62	26.33	26.06	25.86	25.77	25.59
KERO	10.28	11.45	11.36	11.26	11.27	11.17	11.08	11.08	10.98	10.89	10.79	10.79	10.68	10.71	10.61
DIESEL	17.04	18.92	18.93	18.74	18.75	18.75	18.57	18.57	18.48	18.39	18.22	18.23	18.09	18.12	18.13
AGO	4.87	5.47	5.48	5.48	5.38	5.37	5.38	5.39	5.39	5.39	5.38	5.41	5.68	5.39	5.3
ATM-RES	42.28	35.64	35.94	36.52	36.84	37.16	37.73	37.94	38.31	38.81	39.45	39.74	40.11	40.09	40.56
OFF GAS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
VAC-OVHD	0.95	1.04	1.03	1.02	1.01	1	0.99	0.98	0.97	0.96	0.95	0.94	0.932	0.95	0.92
LVGO	8.57	9.16	9.16	9.17	9.27	9.27	9.28	9.28	9.29	9.29	9.49	9.28	9.3	9.24	9.31
HVGO	13.78	13.92	14.03	14.23	14.24	14.34	14.45	14.45	14.56	14.66	14.98	14.65	14.78	14.88	14.89
VAC-RES	77.26	76.34	76.28	76.12	76	75.9	75.8	75.84	75.77	75.67	75.27	75.63	75.5	75.54	75.53
L.GAS	8.224387	8.28202	8.282187	8.282774	8.282858	8.282942	8.283446	8.283446	8.283867	8.307918	8.285894	8.286148	8.287166	8.286487	8.287166
LPG	15.2755	16.69007	16.69418	16.70859	16.71065	16.71271	16.72508	16.72508	16.73541	16.80494	16.78515	16.79139	16.81639	16.79971	16.81639
FCC-GAS	45.48242	41.47497	41.46333	41.42251	41.41668	41.41084	41.37578	41.37578	41.34653	40.3543	41.20561	41.18794	41.11711	41.16435	41.11711
COKE	3.938397	3.965995	3.966075	3.966356	3.966396	3.966437	3.966678	3.966678	3.96688	3.978397	3.96785	3.967972	3.96846	3.968134	3.96846
TGO	27.0793	29.58694	29.59423	29.61977	29.62342	29.62707	29.64901	29.64901	29.66731	30.55444	29.75549	29.76655	29.81087	29.78131	29.81087
SULFUR	0.43	0.455	0.502	0.553	0.602	0.652	0.7	0.749	0.799	0.848	0.897	0.946	0.982	1.021	1.046
API	38.5	34.96	34.81	34.64	34.48	34.32	34.16	34	33.9	33.86	33.77	33.66	33.61	33.45	33.38
VISCOUSITY	4.976	4.073	4.152	4.239	4.322	4.409	4.492	4.634	4.802	4.924	5.077	5.267	5.397	5.59	5.693
CRUDE COST	115.93	115.383	114.836	114.289	113.742	113.195	112.648	112.101	111.554	111.007	110.46	109.913	109.366	109.0925	108.819
PROFIT	28483	35039	36682	37796	39434	40900	42019	43634	44954	46062	47650	48996	50805	50624	51674

%RAT	28	30	32	34	36	38	40	42	44	46	48	50	52	54	56
% BRENT	72	70	68	66	64	62	60	58	56	54	52	50	48	46	44
SCENARIOS	28_72	30_70	32_68	34_66	36_64	38_62	40_60	42_58	44_56	46_54	48_52	50_50	52_48	54_46	56_44
NAPHTHA	25.39	25.21	24.92	24.74	24.53	24.34	24.19	23.96	23.78	23.5	23.21	22.84	22.74	22.55	22.36
KERO	10.61	10.52	10.52	10.43	10.36	10.26	10.27	10.17	10.08	9.98	9.98	9.87	9.79	9.69	9.7
DIESEL	17.93	17.88	17.94	17.75	17.81	17.72	17.03	17.53	17.44	17.35	17.35	17.08	17.17	17.18	16.99
AGO	5.3	5.29	5.31	5.31	5.23	5.23	5.13	5.24	5.1	5.25	5.25	5.21	5.25	5.16	5.16
ATM-RES	40.97	41.29	41.54	42.03	42.61	42.97	43.87	43.7	44.07	44.57	44.87	45.01	45.73	46.11	46.5
OFF GAS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
VAC-OVHD	0.92	0.91	0.93	0.89	0.89	0.88	0.89	0.87	0.86	0.85	0.85	0.75	0.83	0.83	0.82
LVGO	9.31	9.26	9.33	9.33	9.36	9.36	9.36	9.38	9.38	9.39	9.49	9.40	9.39	9.41	9.41
HVGO	14.8	14.78	14.91	15.02	15.16	15.27	15.38	15.49	15.6	15.61	15.72	15.08	15.84	15.75	15.85
VAC-RES	75.61	75.78	75.36	75.49	75.34	75.3	75.24	75.08	74.9	74.99	74.77	74.82	74.83	74.93	74.84
L.GAS	8.287677	8.287166	8.288188	8.288871	8.31499	8.292823	8.27695	8.292996	8.293515	8.317858	8.319301	8.280766	8.320841	8.321477	8.322114
LPG	16.82892	16.81639	16.84147	16.85822	16.97331	16.95524	16.56563	16.95948	16.97222	17.0416	17.07595	16.6593	17.1126	17.12774	17.14291
FCC-GAS	41.08162	41.11711	41.04607	40.9986	39.86937	40.72376	41.8275	40.71174	40.67564	39.67266	39.57371	41.56215	39.46814	39.42454	39.38086
COKE	3.968704	3.96846	3.968949	3.969276	3.981783	3.971168	3.963567	3.971251	3.9715	3.983157	3.983848	3.965395	3.984585	3.98489	3.985195
TGO	29.83308	29.81087	29.85532	29.88503	30.86056	30.05701	29.36635	30.06453	30.08712	30.98473	31.04719	29.53239	31.11383	31.14135	31.16892
SULFUR	1.093	1.142	1.189	1.237	1.284	1.331	1.787	1.425	1.472	1.518	1.52	2.112	1.614	1.661	1.707
API	33.25	33.12	32.99	32.86	32.77	32.66	29.85	32.43	32.3	32.21	32.32	30.98	32.12	32.02	31.93
VISCOUSITY	5.921	6.377	6.821	7.265	7.861	8.178	15.78	9.002	9.443	9.876	9.941	23.48	10.68	11.03	11.33
CRUDE COST	108.272	107.725	107.178	106.631	106.084	105.537	104.99	104.443	103.896	103.349	102.802	102.255	101.708	101.161	100.614
PROFIT	52884	54372	55556	57153	59337	60820	61801	63707	64500	66232	67517	70908	70187	71707	72972

%RAT	58	60	62	64	65	66	68	70	72	74	76	78	80	82	84
% BRENT	42	40	38	36	35	34	32	30	28	26	24	22	20	18	16
SCENARIOS	58_42	60_40	62_38	64_36	65_35	66_34	68_32	70_30	72_28	74_26	76_24	78_22	80_20	82_18	84_16
NAPHTHA	22.06	21.84	21.57	21.29	21.18	21.07	20.89	20.46	20.32	20.13	19.83	19.66	19.23	19.14	18.87
KERO	9.6	9.51	9.51	9.41	9.41	9.3	9.32	9.22	9.12	9.12	9.03	8.93	8.83	8.83	8.76
DIESEL	16.99	16.9	16.8	16.83	16.62	16.61	16.62	16.44	16.33	16.35	16.26	16.21	16.06	16.07	16.01
AGO	5.16	5.16	5.06	5.07	5.07	5.06	5.07	4.99	5.07	5.08	5.08	5.08	5.09	4.98	5
ATM-RES	46.91	47.42	47.8	48.17	48.48	48.67	48.88	49.74	49.99	50.14	50.65	50.96	51.62	51.81	52.39
OFF GAS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
VAC-OVHD	0.81	0.83	0.8	0.79	0.79	0.78	0.78	0.77	0.77	0.77	0.76	0.76	0.75	0.75	0.74
LVGO	9.41	9.41	9.42	9.42	9.43	9.43	9.44	9.55	9.54	9.55	9.55	9.55	9.56	9.57	9.49
HVGO	15.85	15.85	15.87	15.88	15.88	15.89	15.99	16.02	16.02	16.13	16.14	16.24	15.94	16.06	16.21
VAC-RES	74.83	74.91	74.81	74.84	74.87	74.86	74.74	74.48	74.66	74.56	74.54	74.48	74.74	74.65	74.6
L.GAS	8.322296	8.296381	8.323665	8.324123	8.290927	8.32504	8.325132	8.302906	8.302639	8.327158	8.29196	8.29196	8.293169	8.306303	8.30928
LPG	17.14725	16.5303	17.17985	17.19074	16.9087	17.21258	17.21476	17.20272	17.19617	17.263	16.93405	16.93405	16.96372	17.2861	17.35916
FCC-GAS	39.36837	41.14537	39.27446	39.24308	40.8556	39.1802	39.1739	40.02264	40.04119	39.03496	40.78378	40.78378	40.69972	39.78644	39.57946
COKE	3.985282	3.972872	3.985938	3.986157	3.97026	3.986596	3.98664	3.975997	3.975869	3.98761	3.970755	3.970755	3.971334	3.977624	3.979049
TGO	31.17681	30.05508	31.23609	31.2559	29.97451	31.29559	31.29957	30.49573	30.48413	31.38727	30.01945	30.01945	30.07206	30.64353	30.77305
SULFUR	1.754	2.471	1.85	1.898	1.921	1.944	1.99	2.04	2.116	2.126	2.171	2.216	2.26	2.304	2.344
API	31.8	27.36	31.58	31.42	31.36	31.31	31.2	31.08	30.77	30.89	30.8	30.7	30.61	30.52	30.53
VISCOUSITY	11.64	32.26	12.31	12.75	12.99	13.23	13.69	14.16	15.03	15.06	15.43	15.77	16.08	16.35	16.46
CRUDE COST	100.067	99.52	98.973	98.426	98.1525	97.879	97.332	96.785	96.238	95.691	95.144	94.597	94.05	93.503	92.956
PROFIT	73624	75269	74756	75623	75986	75777	77022	76751	77816	78712	79495	80296	80081	80993	81757

%RAT	86	88	90	92	94	96	98	100
% BRENT	14	12	10	8	6	4	2	0
SCENARIOS	86_14	88_12	90_10	92_8	94_6	96_4	98_2	100_0
NAPHTHA	18.62	18.43	18.13	17.93	17.64	17.33	17.05	15.04
KERO	8.66	8.56	8.46	8.47	8.37	8.27	8.26	10.82
DIESEL	15.91	15.82	15.82	15.63	15.53	15.43	15.43	13.69
AGO	4.59	5.01	4.9	4.91	5.01	5.02	5.02	4.27
ATM-RES	53.29	53.27	53.77	54.16	54.56	55.04	55.22	57.79
OFF GAS	0	0	0	0	0	0	0	0
VAC-OVHD	0.73	0.73	0.722	0.72	0.73	0.73	0.73	0.73
LVGO	9.5	9.5	9.51	9.61	9.62	9.62	9.63	9.12
HVGO	16.33	16.45	16.55	16.65	16.67	16.67	16.79	16.83
VAC-RES	74.47	74.37	74.24	74.06	73.91	73.94	73.88	75.34
L.GAS	8.310732	8.310823	8.294295	8.312099	8.312464	8.31338	8.313563	8.221178
LPG	17.3948	17.39704	16.99137	17.42836	17.43733	17.45979	17.46429	15.19671
FCC-GAS	39.47847	39.47215	40.62139	39.38342	39.35801	39.29437	39.28163	45.70562
COKE	3.979744	3.979788	3.971873	3.980399	3.980574	3.981012	3.9811	3.93686
TGO	30.83624	30.8402	30.12107	30.89572	30.91162	30.95144	30.95942	26.93963
SULFUR	2.388	2.438	2.481	2.525	2.568	2.611	2.655	3.88
API	30.44	30.36	30.27	30.18	30.09	29.99	29.89	24.5

VISCOUSITY	16.67	16.82	17.04	17.33	17.55	17.73	17.89	118.8
CRUDE COST	92.409	91.862	91.315	90.768	90.221	89.674	89.127	88.58
PROFIT	81591	82768	83379	83531	83755	83983	84614	84168

Appendix I Publications

Journal Paper

- Edith Ejikeme-Ugwu, Songsong Liu, Lazaros Papageorgiouand Meihong Wang(2012), Development of an Aggregate Model for Refinery Production Planning.(In Preparation)

Peer reviewed conferences

- Ejikeme-Ugwu, E. And Wang, M. (2012) Aggregate Model for Refinery Production Planning In: Ian David Lockhart Bogle and Michael Fairweather (Editors). (eds.) *22nd European Symposium on Computer Aided Process Engineering* (ESCAPE-22). Computer Aided Chemical Engineering, 17 -20 June 2012, London (Accepted).
- Ejikeme-Ugwu, E., Liu, **S.**, and Wang, M. (2011) Integrated refinery planning under demand uncertainty. In: Pistikopoulos, E.N., Georgiadis, M.C., and Kokossis, A.C. (eds.) *21st European Symposium on Computer Aided Process Engineering* (ESCAPE-21). Computer Aided Chemical Engineering, vol. 29. Amsterdam, Elsevier. pp. 950–954.

Presentations

- IChemE CAPE Subject Group PhD Poster Day, University of Leeds, UK, 12 May 2010.
- Ejikeme-Ugwu, E. And Wang, M. (2012) Planning for the Integrated Refinery Subsystems, 9thInternational Conference on Computational Management Science (CMS), 18-20 April 2012Imperial College London (Accepted).