

**LINEAR PROGRAMMING MODELING OF 15 MMTPA  
REFINERY FOR BS-VI AUTO FUELS USING ASPEN PIMS**

*A PROJECT REPORT*

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## **Abstract**

Refineries are one of the most complex industries in the planet. Different kind of units using enormous amount of energy makes it more difficult to handle. Moreover, the global warming has brought an increasing concern towards the emissions of SO<sub>x</sub> and NO<sub>x</sub>. This has lead to optimized refinery planning, starting from the purchase of crude oil to the product supply demand. The refinery planning can be done to generate maximum profit according to the selection of crude oil depending to various factors, to the blending of feedstock to get desired products. The primary objective of this project is to perform a configuration study of a refinery which is currently operating at the production capacity of 15MMTPA. The refinery is generating auto fuels according to the Bharat Stage IV norms developed by Government of India. This project will be the modeling of 15 MMTPA refinery producing BS-IV and BS-VI auto fuels. First the LP model of BS-IV auto fuels will be generated and the input will be manipulated to produce BS-VI grade auto fuels. Two different kinds of crudes will be selected for the project. This will give the idea regarding the quality of the fuels produced from both the cases. The method of linear programming is used to carry out the overall material balances of the refinery, along with the blending of different streams to match the BS-VI specifications of auto fuels. Aspen PIMS by Aspentech Inc. is used for LP modeling in both phases. The solution files for comparison will be available at the end of the completion of the project.

Keywords : linear programming, PIMS, LP modeling, refinery planning, blending

# Table of contents

<b>List of figures</b>	<b>xiii</b>
<b>List of tables</b>	<b>xv</b>
<b>Symbols</b>	<b>xviii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Refinery Planning . . . . .	2
1.1.1 NLP in Refinery Planning . . . . .	2
1.1.2 Multi Refinery Planning Model . . . . .	4
1.2 Introduction to Aspen PIMS . . . . .	4
<b>2 Literature Review</b>	<b>9</b>
2.1 A general sense of linear programming . . . . .	9
2.2 Genetic Algorithms in Multi Objective Planning Model . . . . .	9
2.3 A typical linear programming model . . . . .	10
<b>3 A Crude Fractionation Planning Model</b>	<b>13</b>
3.1 Introduction . . . . .	13
3.2 CDU Fractionation Index Model . . . . .	14
3.2.1 The Model Equations . . . . .	14
3.2.2 Linear Programing - Planning Model . . . . .	16
<b>4 Refinery Fundamentals</b>	<b>19</b>
4.1 Refinery Units . . . . .	19
4.1.1 Crude Distillation Unit . . . . .	20
4.1.2 Naphtha Hydro-Treating Unit (NHT) . . . . .	21
4.1.3 Naphtha Isomerization Unit (ISOM) . . . . .	22
4.1.4 Continuous Catalytic Cracking Unit . . . . .	22
4.1.5 Diesel Hydro Treating Unit (DHDT) . . . . .	23
4.1.6 Hydrogen Generating Unit (HGU) . . . . .	24
4.1.7 Hydro-Cracker Unit (HCU) . . . . .	24

4.1.8	Vacuum Gas Oil Hydro Treater (VGO HDT) . . . . .	26
4.1.9	Delayed Coking Unit (DCU) . . . . .	27
4.1.10	Petrochemical Fluid Catalytic Cracker (PFCC) . . . . .	28
4.1.11	Captive Power Plant (CPP) . . . . .	29
4.1.12	Sulfur Recovery Unit . . . . .	29
<b>5</b>	<b>Refinery Planning Model</b>	<b>31</b>
5.1	Characteristics of the Model . . . . .	31
5.2	Crude Assay Data . . . . .	32
5.3	Sub Units . . . . .	33
5.4	Targeted Product Specifications . . . . .	34
5.5	Base Case Design . . . . .	34
5.6	Alternate Case Design . . . . .	34
<b>6</b>	<b>Petroleum Assay</b>	<b>35</b>
<b>7</b>	<b>Refinery Planning Model in PIMS</b>	<b>39</b>
7.1	Steps in creating a mathematical model . . . . .	39
7.1.1	Problem Recognition . . . . .	39
7.1.2	Collect Information and Data . . . . .	39
7.1.3	Building The Model . . . . .	40
7.1.4	Solving The Model . . . . .	40
7.1.5	Model Validation . . . . .	40
7.1.6	Model Implementation . . . . .	40
7.2	Creating refinery planning model in PIMS . . . . .	41
7.2.1	The Solution . . . . .	41
7.2.2	Components of PIMS . . . . .	42
7.3	The Structure of a Refinery Planning Model . . . . .	42
7.3.1	Rows and Columns Names and Types . . . . .	43
7.3.2	Units of the Row . . . . .	44
7.3.3	Property from other subtables . . . . .	45
7.3.4	Blending Specifications . . . . .	46
7.3.5	Stream Pooling . . . . .	46
7.3.6	Distributed Recursion . . . . .	47
7.3.7	Objective Function . . . . .	48
7.3.8	Interpretation of the Solution Report . . . . .	49
7.3.9	Delta Modeling . . . . .	50

7.4	Crude Distillation Modeling . . . . .	50
7.4.1	ASSAYS . . . . .	50
7.4.2	CRDDISTL . . . . .	51
7.4.3	CRDCUTS . . . . .	53
7.4.4	SCRD . . . . .	55
7.5	Vacuum Distillation Modeling . . . . .	56
<b>8</b>	<b>Results and Discussion</b>	<b>57</b>
8.1	Objective . . . . .	57
8.2	Refinery Configuration : LP Modeling Development . . . . .	59
8.2.1	BS IV Compilant Diesel Hydrotreating Unit . . . . .	59
8.2.2	BS IV Compilant VGO Hydrotreating Unit . . . . .	59
8.2.3	Fluidized Catalytic Cracking Unit . . . . .	59
8.3	Conclusion . . . . .	61

# List of figures

4.1	Hydrocracker Unit . . . . .	25
4.2	Hydro Treater using FCC unit . . . . .	26
4.3	FCC unit . . . . .	28
4.4	Sulfur Recovery Unit . . . . .	29
7.1	CRDDISTL . . . . .	52
7.2	CRDCUTS . . . . .	54
7.3	SCRD . . . . .	55



# List of tables

1.1	Timeline of LP in Refinery Planning . . . . .	2
8.1	Specification of BS-VI MS Regular and Premium . . . . .	58
8.2	Specifications of BS-VI Diesel . . . . .	58

# Symbols

## Subscripts

$fs$	crude oil
$i$	component
$j$	crude cut
$k$	processing unit
$l, l_0$	refinery streams, typically $l$ is a feed to the unit and $l_0$ is an output stream
$p$	refinery product stream
$r$	stream property

## Other Symbols

$T_{ci}, T_{ri}$	critical and reduced temperatures of component $i$
$PB_{j,i}$	bottom product flow rate of component $i$ from fractionation unit $j$ of the $FI$ model
$PV_i$	vapor pressure of component $i$
$C_p$	prices for product stream $p$
$PD_{j,i}$	top product flow rate of component $i$ from fractionation unit $j$ of the $FI$ model
$TI_j, TE_j$	initial and end boiling point temperature values for crude cut $j$
$FST_{fs}$	feedstock $fs$ to the refinery
$K_{j,i}$	equilibrium constant of component $i$ in fractionation unit $j$ (at $T_j$ )
$R_{j,io}$	relative volatility of component $i$ to reference component $o$ in fractionation unit $j$ (at $T_j$ )

$ak, l, l_0, fs$	yield coefficient for output stream $l_0$ for unit $k$ , fed with input stream $l$ associated with crude $fs$
$F_{j,i}$	feed to the fractionation unit $j$ of the $FI$ model, of component $i$
$C_k$	operating cost of unit $k$
$C_{fs}$	cost of feedstock $fs$
$x_{top,i}, x_{bot,i}$	component $i$ composition in the top or bottom product streams of an $FI$ fractionation unit
$FI_j, FI_{rj}, FI_{sj}$	fractionation index of unit $j$ ( $FI_r$ is the value for the rectifying section, while $FI_s$ is the value for the stripping section)
$P_{rr,l,k,fs}$	property of type $r$ of stream $l$ or $l_0$ of unit $k$ and crude $fs$
$T_j$	temperature of the fractionation unit $j$ and also cut $j$
$PR_{r,p}$	property $r$ specification (maximum or minimum) for product stream $p$
$ST_p$	refinery product stream $p$
$ST_{l,k,fs}$	refinery stream $l$ , either as input or as output of unit $k$ , associated with crude $fs$

### **Acronyms / Abbreviations**

CDU	Crude Distillation Column
LP	Linear Programming
MINLP	Mixed Integer Non Linear Programming
PIMS	Process Industry Modeling System
RPMS	Refinery Process Management System

# Chapter 1

## Introduction

Refineries are an important part of energy consumption around the world. A typical refinery consists of the production system which is planned to produce the refining products according to the market demand and the utilities which will provide enough power to run these systems. Today, the petroleum refining industry has reached the pinnacle both in the adoptions of operation research technologies and the developments of software solutions which will tackle the refinery planning problems in the twentieth century.

The supply chain of an oil refining organization comprises of an extensive varieties of activities such as the assessment of crude oil, selection of crude oil for downstream processing, procurement, financial matters pertaining to crude oil selection and processing, transportation of crude oils to the site as well as the scheduling of the refinery operations followed by the transportation of finished products to intermediate terminals and other storage sites.

Optimization is connected at different levels of oil refinery, since economics have a noteworthy impact in these frameworks. For instance, the ideal selection of crude oils is an element of components such as the refiner's location and configuration, seasonal constraints, product specifications, variations in cost of crude oil and products, transportation cost, it's chemical composition and other calculated requirements, for example, accessibility of pipelines and a few different contemplations.

In short, the use of optimization software at the planning level aims to achieve two distinctive goals. The first is to optimize the purchase of a best mix of crude oils and utilities as well as imported products for future planning cycles from month to years of operations. The second goal is to optimize the entire refinery operations starting from distillation cut points, unit throughputs and severity of the conversion units. These applications are tailor made or customized for the operations and planning for refinery operations and supply chain and are used in the refineries for a large scale. Honeywell's RPMS, Ingenious ProPlan and Aspen PIMS are widely used supply chain and production planning applications for refineries.

Table 1.1 Timeline of LP in Refinery Planning

Year	Event
1950s	Invention of simplex algorithm by Dantzig, giving birth to LP
1950s	First Fortran LP code written for refinery optimization
1957	Booner and Moore is the premier refinery LP software provider
1960s	Research and codes are developed in mainframe computers
1960s-1970s	RPMS is written for mainframes and sold by B&M
1980s	Haverly introduces GRTMPS
1981	Aspen Technology is formed
1997	Aspen Technology acquires PIMS
2003	First general purpose MINLP solver is used in Aspen PIMS

The early developments of linear programming started from the birth of simplex algorithms by Dantzig and since then, many LP techniques were constantly emerging and has been applied in the optimization of refinery planning operations.

## 1.1 Refinery Planning

### 1.1.1 Evolution of non linear programming in refinery planning

It is frequently assumed that the refinery planning is as yet based on linear models. Since the late 80s the models have been nonlinear and often mixed integer nonlinear (MINLP) despite the fact that they were still named as linear. The introduction of nonlinear optimization procedure for refinery planning began from 1977 amid an LP instructional meeting at El Segundo refinery. Senior mathematician William "Bill" Hart was working with Don White. He noticed the current models that incorporate multiple yields for various crude oils and operating parameters tended to over optimize the handling and mixing of individual crude oils and their related side-cuts all through the difference in value between the individual crude oils. Amid the session, Hart built up the idea of recursion strategy, which gave an establishment to the work done by Ladson and Joffe, which is called distributive recursion. Distributive recursion gives the basic association between the property or quality changes of the crude oil distillation level with the downstream blending level.

The use of mathematics had been widely used for the long term plant wide refinery planning. Although the accuracy of the results depended on rigorous models, the usage

of these kinds of models were put into use much less due to their complexity. Softwares such as Aspen PIMS, GRTMPS etc. applied the nonlinear recursion algorithm to handle nonlinearities or provide interface to the simulator for planning. The changes in the feed and operating parameter inputs were made to reduce the complexity of the model; using some linear constraints which are available generally and not from refinery data.

To include the product yields and properties of the crude oil distillation in the planning, two main models were represented. The categorization model and the swing cut model. In the former one, the distillation behavior is predetermined by the use of crude assay with an external simulation program. The simulation program determines the yield cuts at a particular temperature and then these data are to be fed in the LP planning model. One drawback of these kinds of systems are the cut points of distillates are predetermined and are not guaranteed to perform in the similar way in real time. Another method called adherent recursion was proposed to optimize cut points. However, these methods were becoming too complex and time consuming to obtain the final results.

Early recursive techniques were slow and difficult, but the evolution of distributive recursion has made the calculations faster and more reliable. The technique became more popular when Basil Associates were acquired by Aspen Technology and with its further development, it was accepted as a standard in LP modeling systems for refinery planning.

In actual plant operations, the crude column is often defined into different kinds of operating modes such as gasoline mode or diesel mode according to different marketing strategies and to combat the demands. Many refineries still use these modes to plan the refinery. Another major problem to tackle is to effectively blend the products into desired constituents. Normally the yields and properties of CDU fractions are calculated by simulation. Then by the specifications of final products, a spreadsheet is created to blend the modes pairwise. Another method is swing cut modeling. For example, a typical CDU gives two distillates. For the adjustments of volume, two pseudo cuts are added. The range of the pseudo cut is defined as a certain ratio on the crude feed bounded by a lower and upper limit.

The issues to be considered in swing cut modeling are the size of swing cuts and the properties of the cut fractions. The size of swing cuts can be expressed either as the volume transfer of feed or by the boiling temperature range. Typically the swing cut is kept wide at first for better distribution of products in the column, and then it can be shortened subse-

quently.

### **1.1.2 Multi Refinery Planning Model**

Based on the characteristics of crudes, a refinery model can be planned. This involves the following steps

- 1. The relationship between the yield and mixing ratio is determined by plant data as well as simulation data. Since the quality of some of the products is difficult to predict such as asphalt, we can use those values by experience. The total yield includes all the light fractions of atmospheric and vacuum distillation, and their relationship by which the different mixing ratios are obtained. If the data is insufficient, rigorous plant simulation is expected to be done and the data can be generated. In a light oil refining, this step can be omitted if there is no requirement of quality for vacuum distillation.
- 2. Since the mixing ratios and the TBP boiling ranges are given, yields of CDU fractions can be calculated by TBP fitting curves. The cutting temperature and cumulative yield of each crude can be obtained by crude oil evaluation data. The final yield of the product can be expressed as a sum of the yield of each crude and the yield of last light fraction can be derived by a difference of the total yield and other light oil products yield. However a light product might be composed of multiple or part of narrow component. The calculations of the property of a certain product is possible by the conversion of component data into the relationship between the cumulative property and the cumulative yield.
- 3. Determine whether the properties of the products conform to the requirements. If not, adjust the TBP boiling ranges of the fractions. In this way the optimized mass of the CDU fractions can be obtained.

## **1.2 Introduction to Aspen PIMS**

PIMS is a most widely used linear programming tool for generating optimal refining and petrochemical industry planning. This tool is used by more than 60% of refiners worldwide and about 40% of petrochemical plants. It's development is rooted back in 1980s and it was the first application which took input using spreadsheet interface.

PIMS is basically used to generate operating production plans for single as well as multiple plants depending on the plant configuration or functions for a single period or multiple period as well. It models the non linear problems using the sequential linear programming approach as well as simulator interfaces that link to rigorous interfaces that link to rigorous simulator models. The plant can be planned according to the throughput as per day, week, month or year.

The software is usually used by:

- Plant operation and production planners
- Feedstock analysts
- Product blenders
- Capital improvement planners
- Back casting analysts
- Corporate merger and acquisition managers
- Engineering and construction, process licensors and consulting companies

The following are some of the uses of PIMS in refineries and petrochemical industry:

- Feed stock selection considering quality, availability and price
- Product slate selection considering quality, availability and price
- Unit operating targets
- Capital improvement studies to simulate material and financial impact of adding new units, new regulations, debottlenecking, different catalysts, varying severities, changing cutting schemes, etc.
- Inventory management
- Multi-period products blend optimization at the planning level
- Turn around planning for unit shutdowns to show how to operate and manage inventory before, during and after unit shutdowns.
- Feedstock allocation and product distribution when multiple plants serving multiple markets are modeled as a region



PIMS use a spreadsheet interface. The data is to be fed in spreadsheet format via applications like MS Office and it calculates and provides us the optimal solution.

The main tables used in PIMS are:

- Assays (Crude distillation)
- Blending
- Sub Models
- Cases
- Supply Demand
- Utilities

## **ASSAYS**

The major four tables in Assays are:

- **ASSAYLIB**

Assay contains the properties of the crude based on the cut points specified by the user. Typically, third party applications such as Crude Manager is used for the crude assay data. Crude Manager gives the physical properties of the crude along with the yield pattern and various cutpoints at a particular temperature. The True Boiling Point (TBP) is generated, which can be used to ascertain various properties of the crude oil.

- **CRDCUTS**

CRDCUTS defines the straight cuts he would want to obtain from the feed crude after being processed by the CDU. The type of crude cut has to be defined here as well.

- TYPE 0 - Gas stream, separated in saturated gas plant
- TYPE 1 - Straight run, atmospheric cut
- TYPE 2 - Atmospheric residue which can be routed to vacuum tower
- TYPE 3 - Straight run, vacuum cut
- TYPE 4 - Swing cut with several dispositions
- TYPE +5 - Swing cut forced to cut immediately above
- TYPE -5 - Swing cut forced to cut immediately below
- TYPE 9 - Deferred cut produced in downstream unit

- **CRDDISTILL**

This table basically contains the details of the crudes being entered into the CDU. It also contains the utilities consumed by the atmospheric and vacuum columns of the CDU. This is also where the user specifies the crudes going in as feed (individual/blend).

- **CRDCUTS**

This is actually an optional table. In this table, the details of a crude blend in case one is being made, is given. Crude blends are basically denoted percentage wise. Either volume or weight basis

**BLNMIX**

In this table, the user defines the mixture of the blends, i.e. the individual components of the blends specified. For example, to make gasoline we blend the naphtha obtained from the various process units along with the straight cut naphtha with reformate and isomerate to prepare the required grade of gasoline.

**BLNSPEC**

In this table, the user defines the property specification of the blends under specification blend type. The properties of the blends of which the specifications are to be met are typically given by the client. Here, the product specification of BS-VI diesel and gasoline norms are to be met in the model.

**BLNPROP**

In this table, the user defines the properties of the streams which are to be blended. Normally, the common properties like TBP, RON, MON, CCR, etc can be fed as data here, in the model.

**SUBMODS**

Sub models are the various process units which will be participating in the refinery. These are considered to be the gray matter of the refinery. PIMS optimized the various sub models accordingly to receive the required product. PIMS decides which sub model is to be used, how much of the capacity of each sub model is and which sub model will be neglected in order to obtain the most optimal solutions with greater margins.

**CASE**

Case tables are used to run the refinery program for two or more different conditions. For

example, Refinery in DHDT and HCU operating at full capacity; Refinery capacity with no naphtha import, etc. Different kinds of cases will be presented in this model for comparison of the output.

### **SUPPLY AND DEMAND**

These are basically buy and sell tables in the refinery. Some of the materials can be imported as well, such as naphtha, fuel oil, etc. The refined and blended products are sold at a particular price per unit weight, which is to be specified in the tables. PIMS will calculate the best optimal pathways of refining the crude and at the same time, will try to balance the economy of the process as desired.

### **UTILITIES**

Utilities such as natural gas, nitrogen, cooling water, air, etc are purchased and will be used for refinery operations. The utilities sold are basically the excess utilities produced by the refinery which is left after the utilities have been used by the subsequent process units of the refinery.

# Chapter 2

## Literature Review

### 2.1 A general sense of linear programming

Linear programming is derived from something which serves which will help to resolve the problem with limited resources among several notions by having the least resources available. These problems can be expressed mathematically in the form of equations which may be linear or non linear in nature, and can be given certain bounds or constraints, within which the solution is expected to be present.

Linear programming is a method of allocating limited resources to achieve a goal such as maximizing profits and minimize costs. It is widely used in the field of economics, military, industrial, social and others. LP is associated with the explanation of a case in the real world as a mathematical model consisting of a linear objective function with multiple linear constraints.

### 2.2 Genetic Algorithms in Multi Objective Planning Model

In general means, the solution of a multi-objective optimization model depends entirely on the preferences made by the decision maker. This decision maker may be a mathematician, scientist or in a typical production plant - a process engineer. Moreover, this depends on the content of the optimization problem. The decision maker is represented by a utility function which agrees to all objective functions in a scalar form. Most of the situations, the global solutions are not considered, but local solutions are more emphasised. As an approach for obtaining the solution, traditional optimization tools, for example - gradient & simplex based techniques turns out to be troublesome in the case of multiobjective problems, and it is often difficult to find the optimum set of points due to the non-convex nature of the problem. Genetic Algorithms, which are stochastic based techniques developed on the concepts of natural evolution, has been found to perform well in the case of multi-objective optimization because of its ability to search for multiple solutions in parallel. Its ability

to handle complex problems with discontinuities, multimodal, discrete and disjoint spaces proves the effectiveness of genetic algorithms in optimization.

The solutions of multiple objective functions differs from that of single objective function in such a way that we will get a series of perfect solutions rather than a normal, single solution. It is called a Pareto set. These solutions are wider than that of the typical single solution and they have proved to be superior to them when all objective functions are taken into consideration.

The genetic algorithm seems perfect for solving multi-objective optimization problems as it generates the entire Pareto sets in a single run instead of performing a series of separate runs and they are less susceptible to change the shape or continuity of the Pareto front. Moreover, some of the key advantages of GA among other techniques for Pareto set approximations are its requirements of its objective function evaluations, population based algorithm and probabilistic transition rules which have less tendency to deviate from the local solution cluster.

Multi-objective genetic algorithm is developed from genetic algorithm, and it can deal among multiple objectives directly. The population change on each iteration depends on genetic operations in effect on the whole population such as selection, crossover and mutation, and these tasks have key effect on the performance of the algorithm. The inherent, parallel and viable utilization of the worldwide data are the principle qualities of this calculation. Eventhough genetic algorithms have proven to be more effective than other optimization methods, the usage of this method is advisable only in a unit problems, such as scheduling of crude oils in a refinery, calculating the optimum parameters of a fluidised catalytic cracking reactor, etc.

## 2.3 A typical linear programming model

A linear programming model consists of the following:

- *Objective function* is the major equation which is linear in nature.
- *Decision variables* are the variables which will take participate in the problem. These variables are to be plotted to check the feasible region.
- *Constraints* are those values which give a limit to the plots of the decision variables. For example, a constraint is so encountered so we can not determine the price when the decision variables are random in order.

- *Limiting signs* explain the variable according to the assumption for the model. It can be positive or negative.

Many approaches has been made through linear and non-linear mathematical means which will make uses of binary variables such as MILP and MINLP codes which proved to be much help in modeling and decision making (Grossmann et al. 2002). Short term scheduling problem for the crude-oil inventory management has been done. The reformulation linearization technology (RLF) in linear programming may lead to the dis-proportionality of composition of crude oil (Kelly & Mann, 2003). The objective function was the minimization of total operating cost, which comprises of unloading cost of crude vessels, inventory cost and changeover cost. Another mixed integer non-linear programming model was developed (Glissmann & Gruhn, 2001) which assumed that a refinery is a complex network consisting of different processing units with an assortment of input/output streams with different properties, which can be blended to desired properties after it's processing in different units of the refinery. Each unit of the refinery is a processing unit which converts a particular stream into desired product. The general model of a typical refinery includes the set of variables such as feed flow rates, feed properties, operating variables, product flow rates and product properties. The use of successive linear programming was used to highlight the importance of optimizing the scheduling an oil-refinery crude feedstock from the receipt of charging pipe stills (Moro et al. 1998).

Blending has been a major challenge in refineries. Blend planning, also called as off-line blending has been addressed by the implementation of several optimization tools. Commercial applications like AspenBlend<sup>TM</sup> and Aspen PIMS-MBO<sup>TM</sup> serves the purpose. On-line blending has been carried out in refineries nowadays, which does optimization during the long run and can change values like price fluctuations. Similar kind of problem was solved by (Tan & Trierwiler, 2001); where a mixed-integer linear programming was used. The proposed strategy for the whole enhancement issue depends on the unraveling the non-linear programming model relating to the answer for the issue, which can be broken down further to solve as MILP scheduling model. This is done only as fixed decisions for optimization in only resource and temporal aspects. It is well clear to understand that most of the uncertainties in the parameters are modeled taking probability distributions into account, which are derived from the generated data. However, for some instances, the data generated is not enough for model the probability distribution and thus are specified based entirely on technical experience.

In a multi-objective optimization, the solution is dependent on the preference of the decision maker, which can be represented by a function which agrees all objective functions

according to the constraints. Both global and local functions are generated of which priority is given to the local functions due to the flexibility in tradeoff analysis.

As for the methodology for approaching the solution, the conventional optimization techniques such as simplex-based methods and gradient-based methods are difficult to find the optimal network due to the non-convexity of the mathematical representation of the problem. It has been proved by extensive research that the use of genetic algorithms for multi objective optimization problems has succeeded in the generation of multiple solutions, but their role in handling discontinuities, multimodal occurings and disjoint spaces have lead researchers and mathematicians to find alternate methodologies for non linear optimization.

# Chapter 3

## A Crude Fractionation Planning Model

### 3.1 Introduction

The component distribution  $i$  at the top and bottom streams, which can be expressed in the molar fractions  $x_{t,i}$  and  $x_{b,i}$  connected to relative volatility  $\alpha_{if}$  of component  $i$  to the reference component  $f$  for the fractionation at total reflux through the following equation:

$$\frac{x_{t,i}}{x_{b,i}} = \alpha_{if}^n \frac{x_{t,f}}{x_{b,f}} \quad (3.1)$$

The above equation uses the minimum number of stages  $n$ , required for the fractionation at total reflux. The straight line which we get when the plotting of the component product composition versus the relative volatility in logarithmic scale, it has been noted that the slope is bounded by two different limiting conditions. Equilibrium flash and minimum number of stages for total reflux fractionation. A single slope means a balanced column with equal power for stripping and rectification. While if it is two slopes means unequal fractionation power in the column. The second slope is called fractionation index (FI). This value changes with the choice of reference components and temperatures used in the calculations. This term can be replaced instead of  $n$  as follows:

$$\frac{x_{t,i}}{x_{b,i}} = \alpha_{if}^{\text{FI}} \frac{x_{t,f}}{x_{b,f}} \quad (3.2)$$

The above equation was used extensively for the crude distillation units. However, the above equation was developed to derive the true boiling point of the streams, all using FI. This method can be done in reverse as well, i.e. to calculate FI from the TBP data. This method has been much easier to calculate TBP data than the available and famous Fenske-Underwood equation.



## 3.2 CDU Fractionation Index Model

The equation provides a simple nonlinear method for calculation of product composition and cut point temperatures in the column without the usage of detailed energy, equilibrium or momentum calculations. The FI values are considered to be the most important characteristic of the unit and its configuration and temperature distribution. This method has the advantage of using Fenske equation and can be used effectively to predict the TBP data of product streams.

To use the model, the complex CDU is divided into a series of simple fractionation units, in which we will know the feed crude oil assay and crude rate, temperature ranges for the cuts. Each unit will have top product and bottom product streams. The top product is fed to the next unit, except to the last unit where it will be the overhead product of the column. The bottom product of each unit is withdrawn as one of the CDU product streams. The overall component balance and mass balance is applied in addition to the FI equation for the equilibrium calculations. The cut point temperature is calculated but it is limited to a particular range, which is normally predefined. This temperature range also defines the range of distributed components seen in both top and bottom products of the unit.

### 3.2.1 The Model Equations

The modeling starts from the mass balance equations. For each cut  $j$  and the component  $i$ , the component in the feed stream  $F$  is related to the unit's top and bottom products, PD and PB as:

$$F_{j,i} = PD_{j,total}x_{PD,j,i} + PB_{j,total}x_{PB,j,i} \quad (3.3)$$

The summation equation of over all components  $i$  for each unit is used as:

$$F_{j,total} = \sum F_{j,i} \quad (3.4)$$

Normally, the light key components (LK) are present in the top stream:

$$PD_{j,i} = F_{j,i}, \quad PB_{j,i} = 0 \quad i < LK_j \quad (3.5)$$

Similarly the heavier key components are only seen in the bottom product stream:

$$PB_{j,i} = F_{j,i}, \quad PD_{j,i} = 0 \quad i > HK_j \quad (3.6)$$

When the composition of the reference components are considered as unity, the boiling point equals the cut point of the cut, the FI equation reduces to

$$\frac{x_{PD,j,i}}{x_{PB,j,i}} = \alpha_{j,io}^{FI}(T_j) \quad (3.7)$$

The above equation combined with the mass balances of previous equations yields the component flow rate in the bottom product stream:

$$PB_{j,i} = \frac{F_{i,j}}{\frac{PD_{j,total}}{PB_{j,total}} \alpha_{j,io}^{FI} + 1} \quad (3.8)$$

$$LK_j \leq i \leq HK_j$$

For the rectifying section where the boiling temperature is lower than the cut point temperature used for the unit ( $T_{b,i} < T_j$ ),

$$PB_{j,i} = \frac{F_{i,j}}{\frac{PD_{j,total}}{PB_{j,total}} K_{j,i}^{FIr_j} + 1} \quad (3.9)$$

$$LK_j \leq i \leq HK_j$$

Similarly for the stripping section where the boiling temperature is higher than the cut point temperature used for the unit ( $T_{b,i} > T_j$ ),

$$PB_{j,i} = \frac{F_{i,j}}{\frac{PD_{j,total}}{PB_{j,total}} K_{j,i}^{FIs_j} + 1} \quad (3.10)$$

$$LK_j \leq i \leq HK_j$$

For the interpretation of the relation between boiling and cut point temperatures  $T_{b,i}$  and  $T_j$ , Heavyside step function can be used:

$$H[x] = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases} \quad (3.11)$$

The following formula yields the implementation of Heavyside step function:

$$FIr_j \frac{1}{1 + e^{4(T_{b,j} - T_j)}} + FIs_j \frac{1}{1 + e^{-4(T_{b,j} - T_j)}} \quad (3.12)$$

The equation will reduce to:

$$PB_{j,i} = \frac{F_{j,i}}{\frac{PD_{j,total}}{PB_{j,total}} K_{j,i} \frac{1}{1 + e^{4(T_{b,j} - T_j)}} + \frac{1}{1 + e^{-4(T_{b,j} - T_j)}}} \quad (3.13)$$

$$LK_j \leq i \leq HK_j$$

The ideal behavior is considered leading to the equilibrium constant  $K$  as:

$$K_{j,i} = \frac{PV_i(T_j)}{P} \quad (3.14)$$

The vapor pressure of the hydrocarbon fractions are calculated using Antoine's equation as:

$$PV_{j,i} = \exp\left(\left(PVA_i - \frac{PVB_i}{T_j + PVC_i - 273.15}\right) 2.303\right) \quad (3.15)$$

The cut point temperature for each cut will be the average or the midpoint between the bounds of initial boiling point and the end boiling point.

$$T_j = \frac{TE_j + TI_j}{2} \quad (3.16)$$

For the vapor pressure calculation of the pseudocomponents, the reduced temperature  $Tr_{j,i}$  will be calculated as:

$$Tr_{j,i} = \frac{T_j}{T_{c_j}} \quad (3.17)$$

The objective of the model when used as a standalone for optimization should be:

$$\max PB_{j,total} \quad (3.18)$$

### 3.2.2 Linear Programing - Planning Model

Other than CDU, all the units to be represented in model will involve the following equation for yield prediction.

$$ST_{l',k,fs} = a_{k,l,l',fs} ST_{l,k,fs} \quad (3.19)$$

The coefficients of these equations are related to the crude oil  $fs$  and the process technology used in each unit. The product stream  $l'$  of unit  $k$  is a function of feed  $l, l \neq l'$ .

Where the product stream is  $l'$  from unit  $k$  and feed  $l$ .

The capacity requirements of different units can be expressed by the inequality as:

$$\sum_l ST_{l,k,fs} \leq capacity_k \quad (3.20)$$

For any model undergoing blending will have splitters and mixers as it is a unit operation. For example, if a splitter splits a single stream called  $l$  into different stream called  $l'$ ,

$$\sum_l ST_{l',sep,fs} = ST_{l,sep,fs} \quad (3.21)$$

Similarly for the mixer which combines the set of streams  $l$  into the single stream  $l'$ ,

$$\sum_l ST_{l',mix,fs} = ST_{l',mix,fs} \quad (3.22)$$

For the product blending units where many blended streams merge to form one product stream  $p$ ,

$$\sum_{l'} ST_{l',k,fs} = ST_p \quad (3.23)$$

For the evaluation of the quality of products, the properties of the streams are necessarily required. They are typically calculated using the linear equations based on the actual values and indices of the properties.

Typically, the specific minimum property of the product will be the sum of the minimum or maximum value of the property. Thus

$$ST_p * PR_{r,p} \leq \sum_{l',k,fs} * ST_{l',k,fs} \quad (3.24)$$

$$ST_p * PR_{r,p} \geq \sum_{l',k,fs} * ST_{l',k,fs} \quad (3.25)$$

The last and the major element will be the profit, which will be calculated from the sales of the final products after deducting the cost of the feedstock and the operating costs of the units.

$$\text{profit} = \sum_p (C_p * ST_p) - \sum_k (C_k * \sum_{l,fs} ST_{l,k,fs}) - \sum_p (C_p * ST_p) \quad (3.26)$$

Where the  $C_p$ ,  $C_k$  and  $C_{fs}$  are price of product  $p$ , operating cost of a particular unit  $k$  which has feed  $l$  and cost of feedstock  $fs$  respectively.

These linear equations used for modeling can be either the fixed yield or swing cut. For a simple refinery configuration, fixed yield is generally used in case the crude is fixed and parameters are not changed.

# Chapter 4

## Refinery Fundamentals

### 4.1 Refinery Units

Different units which are typically present in the refinery are listed as follows:

- 1 Primary  $H_2$ Sing – Crude and vacuum distillation
- 2 Secondary  $H_2$ Sing
  - Fluid Catalytic Cracking (FCC)
  - Hydro Cracking (HCU or OHCU)
- 3 Residue  $H_2$ Sing
  - Delayed coking unit (DCU)
  - LC Fining
  - Vis-breaking (VBU)
  - Bitumen blowing (BBU)
- 4 Treating Units
  - Fuel gas amine treating (FG ATU)
  - LPG caustic wash, ATU and MEROX
  - Naphtha caustic wash, MEROX and hydro-treating
  - MS selective hydro-treating, benzene saturation and isomerisation
  - Kerosene/ATF MEROX, extraction, hydrotreater
  - Diesel hydro-treating (DHDS, DHDT)
  - VGO hydro-treating (VGO HDT)
  - RCO hydro-treating (ARDS)

- Vacuum residue hydro-treating (VRDS)

## 5 Others

- Sour water stripping (SWS)
- Amine regeneration unit (ARU)
- Sulphur recovery unit (SRU)

## 6 Lube Units

- Solvent extraction (SEU)
- Solvent de-asphalting (SDA)
- Solvent de-waxing (SDU)
- Wax de-oiling
- Lube/wax hydro-treating

### **4.1.1 Crude Distillation Unit**

The main equipments which are part of the CDU are:-

- De-salter
- Heater
- Atmospheric Distillation Column (ADU)
- Vacuum Distillation Column (VDU)

Crude distillation typically occurs at temperatures less than 900 degree Fahrenheit (482 °C) at atmospheric pressure. At higher temperatures, cracking starts to occur. To further process the ADU bottoms, we attach VDU. Distillation process is carried by either increasing temperature or decreasing pressure. Since in VDU we cannot further increase the temperature (else cracking starts), we decrease the pressure by the use of vacuum.

In this unit, the process of distillation takes place in which crude oil separates into different fractions according to their boiling points. The cut points taken for this model were:-

- 1 Light ends – NC1, NC2, NC3, NC4, and IC4
- 2 Light Naphtha – 90 °C

- 3 Heavy Naphtha – 90 to 125 °C
- 4 Naphtha/kerosene swing – 125 to 140 °C
- 5 Kerosene – 140 to 197 °C
- 6 Kerosene/diesel swing – 197 to 250 °C
- 7 Light diesel – 250 to 340 °C
- 8 Heavy diesel – 340 to 360 °C
- 9 Diesel/VGO swing – 360 to 375 °C
- 10 VGO (vacuum gas oil) – 375 to 555 °C
- 11 Vacuum residue – beyond 555 °C

#### **4.1.2 Naphtha Hydro-Treating Unit (NHT)**

The naphtha hydrotreater ordinarily pre-treats the naphtha streams preceding being handled in the Catalytic Reforming Unit (CCR) and the Isomerization Unit. The Naphtha Hydrotreater Unit evacuates contaminants, for example, sulfur, nitrogen, and oxygen by advancing hydrogenation reactions (i.e. expansion of hydrogen to the hydrocarbon chain) in a fixed bed reactor containing nickel/molybdenum-advanced aluminum catalyst. Streams of fresh naphtha is input to the Naphtha Hydrotreater Unit from the Crude Distillation Unit, the Diesel Hydro-treating Unit and the Delayed Coking Unit. The blended liquid state naphtha streams are blended with reuse and make-up hydrogen. The feed which are combined enters the reactor encourage/emanating exchanger, where the sustain is warmed. The warmed encourage is raised to the response temperature in a nourish charge radiator. The hot nourish streams down through a fixed catalyst bed. The hydrogen responds with the sulfur and nitrogen contaminants to deliver hydrogen sulfide and  $NH_3$ . Some of this hydrogen sulfide and  $NH_3$  is caught up in a water wash segment only downstream of the reactor. The subsequent sour water item is gathered in a separator and sent to the a sour water collection system.

Presently, the hydro-treated sweet naphtha is sent to the naphtha splitter. It is then fractionated out into off gas and naphtha of different grades. The light and heavy naphtha are sent to the isomerization and catalytic reforming unit separately for further treatment.



### 4.1.3 Naphtha Isomerization Unit (ISOM)

The isomerization unit forms the light naphtha to eliminate benzene by changing over it into cyclo-hexane and to deliver an important product called isomerate which is a vital piece of the blend in gasoline. It is so since this unit expands the octane number of the light naphtha stream.

Hydro-treated Light naphtha stream is charged to one of two dryer vessels. These vessels are loaded with molecular sieves that expel water and ensure the quality of products and catalysts. The feed is heat treated against the reactor exit stream before entering a heater. It then blends with makeup  $H_2$  and is gone through two fixed bed catalytic reactors in a series arrangement.

The reactor exit stream is cooled before entering the product stabilizer. The makeup  $H_2$  is given by CCR. The reactor emanating is isolated in the stabilizer fractionation segment into fuel gas and isomerate. The fuel gas stream is scathing cleaned for expulsion of any  $HCl$  shaped from natural chloride added to the reactor feed to keep up ideal catalyst movement. Subsequent to cleaning, the overhead gas is steered to the gas plant for further handling. The settled isomerate item from segment base is cooled in an air/trim cooler and directed to storage for use in gasoline mixing. The isomerate item for the most part has a RON of around 83 to 85.

### 4.1.4 Continuous Catalytic Cracking Unit

The catalytic reforming unit forms the heavy naphtha to make it more appropriate for blending procedures to make gasoline. The procedure of reforming includes the artificial re-arrangement of the hydrocarbon atoms to deliver higher octane products. Hydrogen gas is a by-product of reforming, it is utilized as sustain to the Naphtha hydro-treating unit, diesel hydro-treating unit and isomerisation unit.

The heavy naphtha stream as feed is blended with recycled hydrogen, preheated by trade with reactor exit stream, warmed to appropriate temperature in the charge radiator and sent to the first of a progression of three to four reactors. Every reactor is gone before by a gas-fired feed radiator to keep up a steady delta temperature profile for the individual reactors. The reformate item is fractionated in the debutanizer for division of light closures, which are sent to the Gas Concentration Plant for recuperation. The reformate (fluid item) is sent to storage, for use in gas oline mixing.

The Catalytic Reforming Unit reactor catalyst is ceaselessly recovered in the Catalytic Reforming Unit Catalyst Regenerator. The recovery segment of the reformer gives a persistent stream of clean without coke active catalyst that is returned back to the reactors. Constant

dissemination of recovered catalysts keeps up ideal impetus execution at high severity conditions for long on-stream times of reforming operation.

Catalyst recovery happens in a controlled environment and utilization of nitrogen, air, and perchloroethylene as recovering resources. The Catalyst Regenerator performs two foremost capacities - strong catalyst recovery and flow. Spent catalyst from the last Catalytic Reforming Unit reactor vessel is passed on to the Catalyst Regenerator, where it is recovered in four stages:

- Burning of coke with oxygen
- Oxychlorination reaction with oxygen and chloride
- Drying of catalyst with air/nitrogen
- Catalyst reduction to higher oxidation states

The regenerated catalysts are hence transferred to catalytic reforming units for further reforming.

#### **4.1.5 Diesel Hydro Treating Unit (DHDT)**

The Diesel Hydro-treating Unit decreases the levels of sulfur and different contaminants in diesel fuel items to meet administrative normalizations. The diesel feedstocks, including straight-run diesel streams from the Crude Distillation Unit and gas oil streams from the base preparing units, are blended with reused hydrogen and heated to the desired temperature in a fired heater.

Hydrogen sulfide and ammonia byproducts are evacuated in the water wash area and an amine contactor downstream of the reactor. The aqueous wash containing some hydrogen sulfide and ammonia is evacuated in a separator, and steered to the sour water system. The  $H_2S$ -rich amine from the contactor is recovered before being come back to the recycle gas scrubber as lean amine. The sweetened gas from the amine absorber is reused back to the recycle gas compressor at the reaction section inlet. A surge of  $H_2$ -rich gas through makeup gas compressor meets the feed stream.

Fluid natural effluent from the reactor is redirected to a stripper where distillates and unstabilized naphtha are isolated. Unstabilized Naphtha is directed to a stabilizer to expel light end hydrocarbons, which are steered to the LPG treating plant for preprocessing and setabilized naphtha is further handled.

The stripper bottoms are isolated into naphtha, kerosene, and diesel parts in a fractionator section. Naphtha is expelled as an overhead stream and sent for further treatment. The hydro-treated kerosene and diesel streams are sent to capacity for mixing operations.

#### 4.1.6 Hydrogen Generating Unit (HGU)

The Hydrogen Generation Unit configuration depends on catalytic reforming and pressure swing adsorption (PSA) framework is to create 99.9 mole % unadulterated hydrogen gas. Hydrogen is created by steam reforming of Re-gasified Natural Gas/Naphtha. LNG from surge drum is pumped to the LNG vaporizer. Vaporized LNG subsequent to blending with reused hydrogen and superheated steam enters the pre-reformer. Superheated steam is added to modify the steam-carbon proportion, and the blend is warmed. The superheated nourish steam blend is dispersed through multi-tubular reactor comprising of high amalgam reformer tubes containing nickel-based impetus. Improving responses produces CO,  $CO_2$  and  $H_2$ , and warmth for the endothermic response is provided by various burners with PSA cleanse gas and refinery fuel gas/naphtha as fuel.

The gas which is reformed is subsequently cooled is sent to shift conversion via shift converters. These are barrel shaped settled bed reactors containing iron/chromium oxide or copper/zinc oxide catalysts. Shift conversion responds by changing over the majority of CO into  $CO_2$  and  $H_2$  in nearness of the catalyst. The warmth expelled from the changed over process gas is utilized to vaporize and additionally warm up catalyst, and preheat evaporator nourish water and de-mineralized water (make-up). Downstream of Shift convertor is  $H_2S$  Condensate Separator where condensate is isolated and steered for BFW development and steam.  $H_2S$  gas is sanitized to evacuate inactive gas polluting influences like  $CO_2$ , CO,  $CH_4$ ,  $N_2$  and water vapor by high-weight adsorption of these debasements on sub-atomic strainers, dynamic carbon and alumina gel in Pressure Swing Adsorption (PSA) network. All adsorbed gasses are expelled amid desorption and recovery of the beds, and utilized as reformer burners fuel.

#### 4.1.7 Hydro-Cracker Unit (HCU)

$H_2S$  scheme consists of two stage reactors with recycle. The first stage partially converts the feed blend to diesel and lighter products and the unconverted oil is sent to second stage. The second stage operates in the absence of  $NH_3$  and  $H_2S$ , therefore the relevant kinetic rate constants are much higher than in the first stage. Thus, the second stage operates at lower temperatures, which greatly favors aromatic saturation and reduces hydro-cracking to light-ends and naphtha, resulting in improved selectivity towards middle distillates and better product qualities. Heat released during exothermic reactions is controlled by quench gas injection between reactor beds. Hot HP Separator, Cold HP Separator, Hot LP Separator & Cold LP Separator has been considered. This configuration allows better heat integration

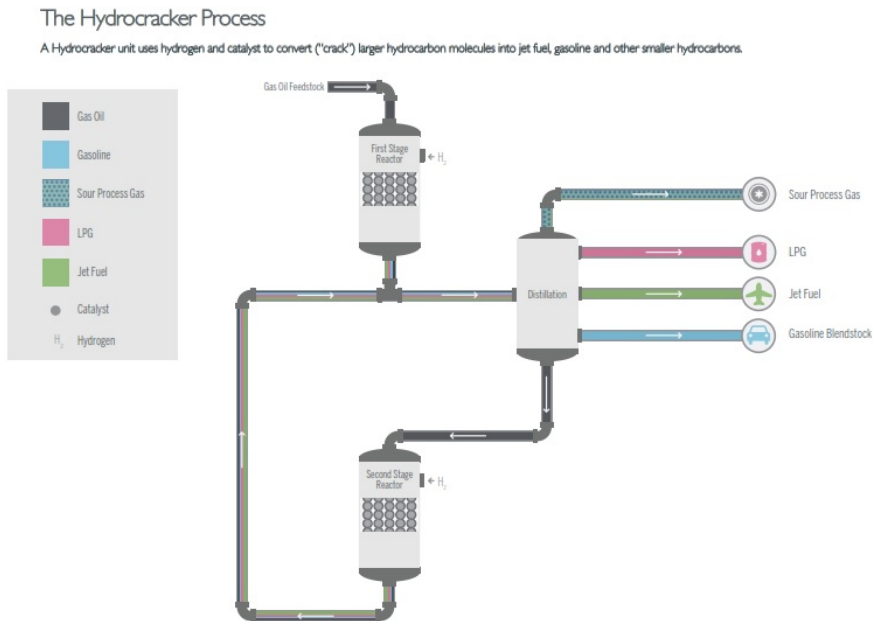


Fig. 4.1  
Hydrocracker Unit [Source - Enerprocess]

between Reactor effluents and feed preheat thus effectively leading to a reduction in fuel firing in reactor charge furnace.

An HP amine scrubbing  $SO_2$  to remove  $H_2S$  from recycle gas is considered. Part of the recycle compressor discharge gas is routed to the reactors as quench and remaining is combined with hydrogen from the make-up hydrogen compressors to form reactor feed. The reactor feed gas splits with part of the gas going to the first-stage reactor and the remaining gas is sent to the second stage. The liquid products from the HLPS and the CLPS are fed to product stripper where column overhead is partly refluxed back to column and partly sent to the gas section along with reflux drum vapor phase. The stripper bottoms feeds the product fractionators where overhead vapor is totally condensed and is routed either back to the product fractionator as reflux or to the gas section. The kero and diesel fractions are routed to side strippers where part is recycled back to the column and part is obtained as kero and diesel products. The fractionator bottoms returns to the reaction section as feed for the second stage.

Gas section feed flows to the de-ethaniser feed drum and pumped to de-ethaniser at the top of the column as reflux. In the Absorber, lean oil is contacted with the overhead vapour stream from the de-ethaniser reflux drum remove  $C_3$  and heavier molecules from the sour gas. The liquid mixed with the unstabilized light naphtha from the product stripper. The overhead

vapour from Absorber is sent as sour fuel gas, Bottoms is pumped by absorber reflux pumps and returned to Column. The bottom product from de-ethaniser mixes with heated overhead naphtha from the product fractionators and enters the debutanizer, hydrocarbon stream from Debutanizer is sent either to the column as reflux or as sour LPG to the LPG treating section for propane and butane recovery and sweetening. The debutanizer bottoms via guard bed feed the naphtha splitter where light and heavy naphtha are separated.

#### 4.1.8 Vacuum Gas Oil Hydro Treater (VGO HDT)

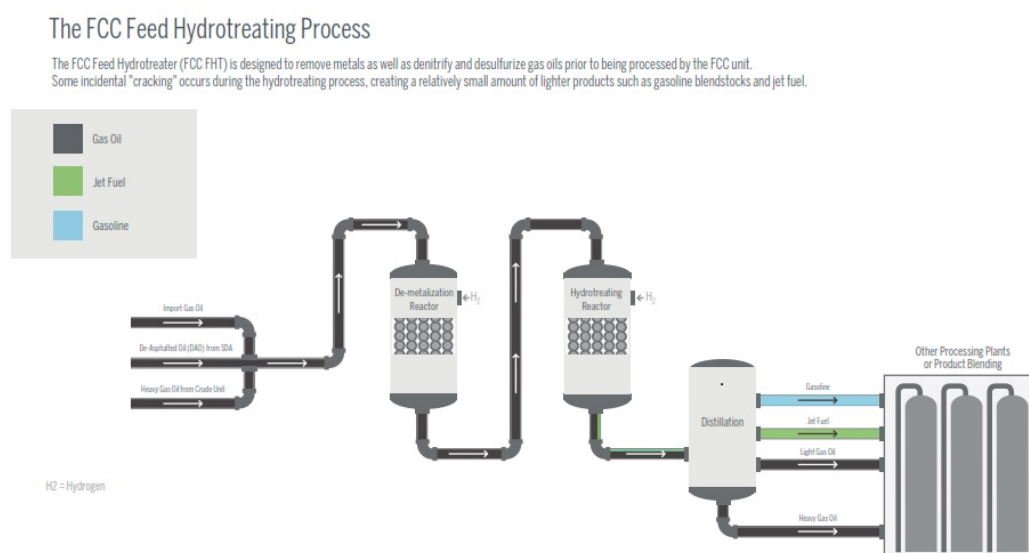


Fig. 4.2  
FCC Hydrotreater [Source - Enerprocess]

A VGO HDT basically treats the LVGO and HVGO from the CDU/VDU and gas oils from the bottom processing units. Fresh feed is preheated, pumped and mixed with the preheated recycle gas. The mixture is brought up to reaction temperature by the reaction furnace. In the reactors the reactions are highly exothermic; therefore, the temperature at the inlet of each bed is controlled by a quench gas injection. The reactor effluent is then fed into the hot HP separator drum.

The vapor phase from hot HP separator is cooled and water is injected at the inlet of the air cooler. The air cooler effluent is collected in the cold HP separator drum where three phases are separated. The sour water is removed and routed to the sour water stripper system. The gas phase is sent to the recycle gas HP amine absorber where almost all H<sub>2</sub>S

is removed. The recycle gas is separated in two parts, one towards quench and the other one with makeup gas to feed effluent exchanger. The hydrocarbon liquid phase from the cold HP separator drum is routed to the LP separator. At LP separator, the hydrocarbon liquid phase is combined with hot HP separator liquid phase and routed to the inlet of the stripper where stripping is ensured by injection of medium pressure steam at the bottom of the column. The overhead vapors from the stripper is partially condensed by air and cooling water and collected in the reflux drum. The liquid hydrocarbon phase is used part as reflux to the stripper and part is sent for gas recovery.

LP separator vapor phase and stripper reflux drum vapor and liquid streams are routed to De-ethanizer via De-ethanizer feed drum. De-ethanizer bottom combines with Fractionator reflux drum liquid phase to feed Debutanizer. Debutanizer overhead vapor are totally condensed and part is routed back to column and net distillate is pumped as LPG. The purpose of Absorber is to maximize LPG recovery which is achieved by counter flow of cooled naphtha coming from Debutanizer bottom. Absorber overhead vapor go to LP amine absorber from where sweet gas is obtained.

#### **4.1.9 Delayed Coking Unit (DCU)**

The Delayed Coking Unit processes vacuum residue. It uses a thermal cracking process to produce lighter liquid products and solid coke. It is a semi-continuous process and employs two parallel coke drums. These coke drums are alternately switched on-line and off-line after filling with coke. The feed enters the bottom of the coker main fractionator where it mixes with condensed recycle material in the column. The combined stream is heated in one of the gas-fired coker charge heaters to initiate coke formation in the corresponding coke drum. Coke drum overhead vapor flows back to the coker main fractionator. This column separates the coke drum overhead vapor into various light hydrocarbon constituents to be returned to other refinery process units. These include coker naphtha, light coker gas oil and heavy coker gas oil.

After coking reactions are complete, the full coke drum is switched off-line and is steamed out and cooled. (The other coke drum is brought on-line and the coking process continues in that reactor train.) Vapors emitted from the opened coke drum are captured by the enclosed blow-down system and are recovered in the main fractionator. When cool, the coke drum bottom and top heads are removed. The coke is cut from the drum with a water jet and dropped into the Coke Pit. Petroleum coke from the Delayed Coking Unit is dropped into the Coke Pit where free water is separated from the coke and recycled. A bridge crane is used to transfer the moist coke from the Coke Pit to the Coke Pad, where it is stored in piles for further dewatering. A bridge crane is also used to transfer coke from the Coke Pad to the

Coke Crusher. The crushed, moist coke is then transferred via an enclosed belt conveyor to the Coke Silos. Coke from the Delayed Coking Unit is transferred via an enclosed belt conveyor to the Coke Loading Facility. This  $SO_2$  includes coke storage silos and a coke railcar loading operation.

#### 4.1.10 Petrochemical Fluid Catalytic Cracker (PFCC)

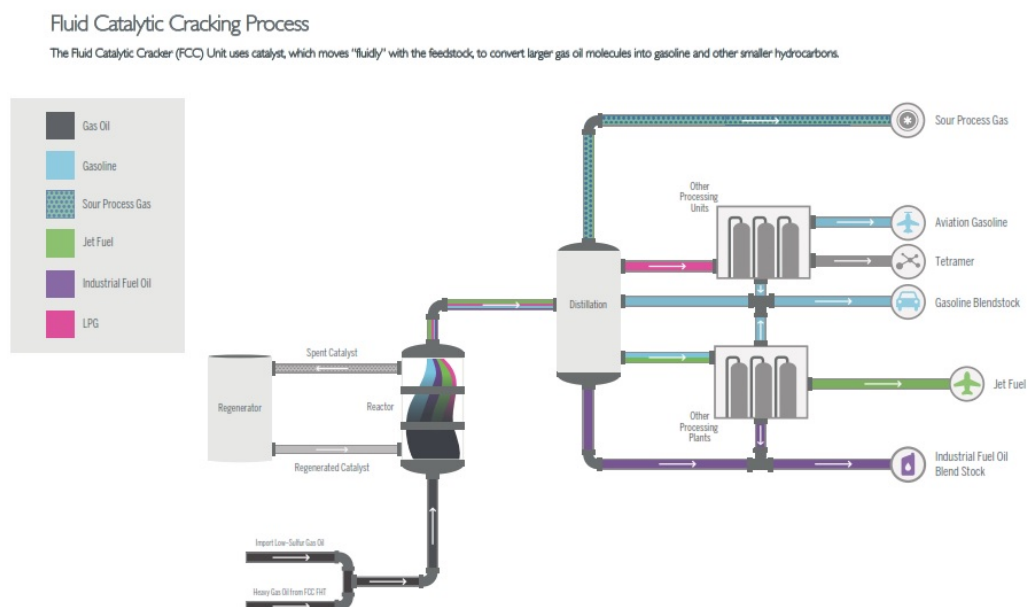


Fig. 4.3  
FCC [Source - Enerprocess]

Petrochemical FCC is a fluidized catalytic process for selectively cracking a variety of feed stacks to light olefins. PFCC is similar to conventional FCC in terms of basic process employed. But the conversions are higher in PFCC. The objective of PFCC is maximization of LPG with higher selectivity towards propylene. LPG yield is typically 37-40% and propylene is typically 20%. Propylene is recovered from LPG in downstream PRU and sent to the polypropylene unit. There is potential to use the dry gas rich in ethylene for the production of styrene monomer after reacting with benzene to form ethyl benzene.

The PFCC gas recovery section employs a low pressure drop main fractionator design with warm reflux overhead condensers to condense the large amount of steam used in the cracker. The absorber and stripper columns, downstream of the wet gas compressor are specifically designed for enhanced C3 recovery at relatively gasoline rates. In addition to the above three products, the product fractionator separates the catalytically cracked material into

heavy naphtha, light and heavy cycle oils and catalyst slurry. The heavy cycle oil is recycled back to the reactor. The catalyst slurry contains some lighter hydrocarbon oil, clarified oil, which is subsequently separated and may be recycled back to either the reactor or to the internal fuel oil pool. The flue gas handling system downstream of the PFCC regenerator requires considerations no different than those of an FCC system. It consists of a flue gas slide valve to control the differential pressure between the reactor and regenerator followed by an orifice chamber. Heat is recovered by flue gas cooler in the form of high-pressure superheated steam.

#### 4.1.11 Captive Power Plant (CPP)

Captive power plant is basically a power generation plant. It uses steam or gas powered turbines to generate electricity for the plant using internally produced fuel gas and fuel oil. This plant increases the self sustainability of the plant for its power needs and reduces its dependence on power from other power generating entities. Conditions like power outages and trips do not occur hence, production from the plant is not hampered.

#### 4.1.12 Sulfur Recovery Unit

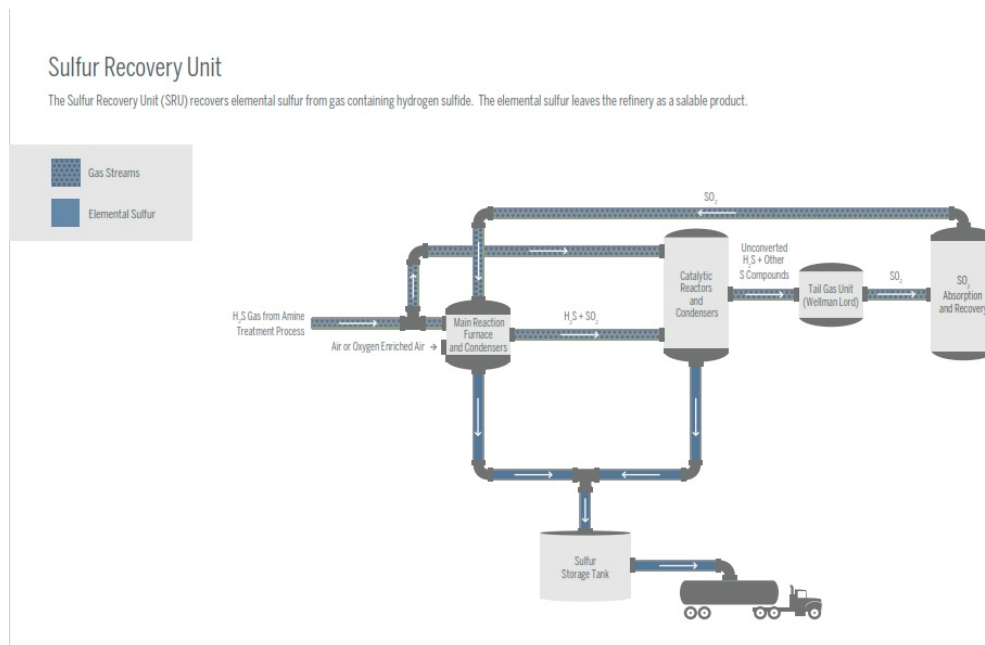


Fig. 4.4  
 Sulfur Recovery Unit [Source - Enerprocess]



The separated High Sulfur containing stream is sent from the amine regenerator to sulfur recovery units, where it is turned into elemental sulfur, using a process known as the “Claus  $H_2S$ ”. Some  $H_2S$  is burned or oxidized in a furnace, creating sulfur dioxide ( $SO_2$ ) from the  $H_2S$ . The  $SO$  produced further reacts with the unreacted  $H_2S$  to produce elemental sulfur. The second step, which produces the elemental sulfur, occurs partially in the reactor furnace and partially in the catalytic reactors. The gases that exit the reactor furnace are routed to a heat exchanger where the elemental sulfur produced in the burner/furnace is condensed and sent to storage. The heat exchanger produces steam for use in the  $SO_2$ . The gases from the heat exchanger are sent to a vessel that contains a catalyst to continue the conversion S to elemental sulfur. The process at the  $SO_2$  has two conversion stages to produce the majority of the elemental sulfur. The process gas that still contains unconverted H of the  $H_2S$  is routed to the equipment called the Wellman-Lord tail gas recovery units, where remaining  $H_2S$  is oxidized to  $SO$  and returned to the catalytic reactors for further conversion to elemental sulfur. The elemental sulfur that is produced is stored in a tank in a liquid form. It is shipped out of the  $SO_2$  as a salable product in liquid form by truck.

# Chapter 5

## Refinery Planning Model

A typical refinery planning problem can be considered as a optimization problem with multiple periods in which the refinery is to be operated at a steady state. Some of the scenarios in real time optimization is the blending problem, where the refiner needs to choose the optimum composition of product streams, which in turn depends on a variety of parameters such as economics, operating modes of refineries, unit capacities, product demand, etc. These are typically solved by linear programming (mixed integer non linear programming)

The following topics will be covered in this chapter:

- Characteristics of the model
- Crude Assay Data
- Sub units and it's specifications
- Targeted Product Specifications
- Base Case Design
- Alternate Case Design
- Case Comparison
- Conclusions

### 5.1 Characteristics of the Model

The refinery model is proposed to have a production capacity of 15 Million Metric Tonnes Per Annum (15 MMTPA). The crude oil which will be used for the model is Arab Heavy. The crude assay of both crudes will be submitted at the end of the project. Utilities such as steam and refined LNG will be purchased at a particular cost, and additional power needed to run the plant can be imported.

## 5.2 Crude Assay Data

The crude oil assay is a compilation of laboratory and pilot plant data that define the properties of the specific crude oil. The assay should contain data on distillation curve for the crude and a specific gravity curve at least. However, most assay contains data on pour point, sulfur content, viscosity and many other properties. Engineering companies develop the assay data of different crudes which they will be using for refining, mostly generated from third party softwares such as SimSci Spiral, or crudes which will be used to work on for a long time, or crudes which are common enough. Some of the data on the crude assay is summarized below.

1. *The true boiling point curve* is a plot of the boiling points of almost pure components, contained in the crude oil or fractions of the crude oil. In earlier times, this curve was produced in the laboratory using complex batch distillation apparatus of a hundred or more equilibrium stages and a very high reflux ratio. Now these curves are produced by mass spectrometry techniques much quicker and more accurately than by batch distillation.
2. *The ASTM distillation curve* is used however on a routine basis for plant and product quality control. This test is carried out in a simple arrangement of distillation flask alongwith condensers to find out the true boiling point of the crude fractions obtained from crude oil. Because only one equilibrium stage is used and no reflux is returned, the separation of components is poor. Thus the initial boiling point (IBP) for ASTM is higher than the corresponding TBP point and the final boiling point (FBP) of the ASTM is lower than that of the TBP curve.
3. *API gravity* is an expression of the density of an oil. API gravity refers to density at 60F. Its relation can be shown by the expression

$$\text{API}^\circ = \frac{141.5}{\text{sp.gr.}} - 131.5 \quad (5.1)$$

4. *Flash point* of the oil is the temperature at which the vapor above the oil will momentarily flash or explode. This temperature is determined by laboratory testing using an apparatus consisting of a closed cup containing the oil, heating and stirring equipment, and a special adjustable flame. Pensky Marten apparatus is used for middle distillate

as a fuel and for kerosene, Abel's apparatus is used. The expression for flash point is represented by:

$$\text{Flash Point} = 0.77(\text{ASTM } 5\% \text{ } ^\circ F - 150^\circ F) \quad (5.2)$$

5. *Octane number* is a measure of a gasoline's resistance to knock or detonation in a cylinder of a gasoline engine. The higher the resistance, the higher will be the efficiency of the fuel to produce work. The anti knocking characteristics of gasoline helps in the judgement of the compression ratio of the engine which it is used in. The higher the octane number of the fuel, the higher the compression ratio of the fuel.

Likewise there are more properties such as viscosity, cloud and pour points and sulfur contents.

There are some of the terms used in the crude oil analysis. They are as follows:

*Cut point* is defined as the range of temperature at which a desired value of the crude fraction is obtained, as found in the upper and lower TBP points. For example, A fraction with an upper cut point of  $100F$  produces a yield of 20% volume of the whole crude as that fraction. The next fraction has a lower cut point of  $100F$  and an upper one of  $200F$  represents a yield of  $30 - 20\% = 10\%$  volume on crude.

*End point* is the actual temperatures which can define the yield of a fraction. When the two fractions are separated in a column, some of the light components remains accumulated in the light fraction. In the same way, some of the heavier components of a particular crude fraction remains with the heavier fraction. In this way, the actual initial boiling point of the fraction will be less than the lower cut point and its final boiling point will be more than the final cut point.

### 5.3 Sub Units

Sub units are the building block of the refinery. In refinery planning, sub units are actually the intermediate processing units which generate desired products based on the specifications and conditions of the feed. Some of the units have been explained in the previous chapter. The following will be the sub units included in the model.

- Naphtha Hydro Treater (NHT)
- Hydrocracker (HCU)
- Petrochemical Fluid Catalytic Cracking Unit (PFCC)

- Visbreaker Unit (VBU)
- Delayed Coker Unit (DCU)
- Diesel Hydro Treating Unit (DHT)
- Isomerization Unit (ISOM)
- Gas Oil Desulfurization Unit (GOHDS)
- Merox Units

## **5.4 Targeted Product Specifications**

The final blended products are always monitored to match the specifications according to different environmental norms such as Bharat Stage or Euro. Here the main aim is to produce HSD VI which has a least amount of sulfur (8 ppm). Motor Spirit (MS) will also be blended using Naphtha from various units. Kerosene will be blended as domestic grade and export grade, with different specifications. Heavies from different units will be blended as fuel oil. The detailed product specifications is given in Bharat Stage VI norms released by Govt. of India.

## **5.5 Base Case Design**

Base case is a foundation of an LP refinery model. Base case is created by keeping all constraints of the equations as open and allowing the model to obtain the optimized set of values. The behavior of the base case determines the performance of the model. Huge amount of data is needed to create the base case and the cases can be altered from the base case according to the requirement of the refiner. The properties of the base case and the altered case will be reviewed at the end of the project.

## **5.6 Alternate Case Design**

The following are the altered cases which will be included in the model for comparison:

- Base Case with FCC Gasoline Treatment Unit
- Base Case with VGO Hydrotreater Unit

# Chapter 6

## Petroleum Assay

Petroleum is a naturally occurring complex mixture of hydrocarbons available in a liquid state and consists of major elements such as hydrogen, carbon, sulfur, nitrogen, etc. It has wide variety of constituents depending on the place of its origin and it shows a wide variations in behavior in refining as well as product specifications. Since the petroleum obtained from different places have varying quantity of sulfur, it has been increasingly difficult for the refiners to process them and produce products with less sulfur content. Thus the process units in a refinery always needs analytical test methods which can adequately evaluate feedstocks and monitor product quality.

Attempts have been made to declassify petroleum based on the various distillation properties when combined with another important property such as density. Such a classification according to the chemical composition at 250-300°C is shown below:

Paraffinic	Naphthenic	Aromatic	Wax	Asphalt	Crude oil Classification
%	%	%	%	%	%
>46 <61	>22 <32	>12 <25	<10	<6	Paraffinic
>42 <45	>38 <39	>16 <20	<6	<6	Paraffinic-naphthenic
>15 <26	>61 <76	>8 <13	0	<6	Naphthenic
>27 <35	>36 <47	>26 <33	<1	<10	Paraffinic-naphthenic-aromatic
<8 >57	<78 >20	<25	<0.5	<20	Aromatic

An efficient assay is derived from a series of test data which gives an accurate description of petroleum quality and helps us to judge its behavior during its processing. Typically two different analytical schemes are commonly used, which are inspection assay and comprehensive assay. Inspection assay normally involves several important parameters such as API gravity, sulfur content, pour point and distillation range, etc. They are means of determining whether major changes will be present if the comprehensive assay will be performed.

A comprehensive assay is more complex than the inspection assay. They are time consuming and costly and they are usually performed only when a new field comes on stream,

or when the inspection assay indicates that the significant changes in the composition of the crude oil has been occurred. Some of the major characteristics in a comprehensive assay will be given below:

- **Carbon residue and Asphaltene content**

The carbon residue of petroleum and petroleum products serves as an important indication of the carbonaceous materials present in the petroleum which will be in effect under the influence of heat. Mainly Conradson carbon residue, Ramsbottom carbon residue, microcarbon residue and asphaltene content are sometimes included in the inspection data of petroleum. The determination of *carbon residue* of petroleum is applicable to relatively non volatile samples that decompose on distillation at atmospheric pressure.

- **Specific gravity**

Specific gravity is an important property of petroleum products because petroleum and petroleum products are purchased and sold most in terms of volume basis, and they are converted to mass basis by use of specific gravity. This property is almost called as density as both terms called density and specific gravity are related to each other. Usually hydrometer, pycnometer or more digitally controlled density meter are used for determination of specific gravity.

- **Distillation**

The distillation tests gives an indication of the type of products and the quality of products which can be obtained from petroleum, and the tests are used to compare different petroleum types through the yield and quality of 300 degrees of residuum fraction. Usually seven fractions provide the basis for detailed distillation properties of the feedstock:

- Gas, boiling range: <15.5 °C
- Gasoline, boiling range: 15.5 - 149 °C
- Kerosene, boiling range: 149 - 232 °C
- Gas Oil, boiling range : 232 - 343 °C
- Light Vacuum Gas Oil : 343 - 371 °C
- Heavy Vacuum Gas Oil : 371 - 566 °C
- Residuum : >566 °C

- **Light Hydrocarbons**

The amount of the individual light hydrocarbons in petroleum is often included as a part of the petroleum assay. They consist mainly of light ends such as methane, ethane, etc and its determination is best carried out by gas chromatographic method.

- **Metallic Constituents**

Petroleum as recovered from the reservoir contains many metallic and non metallic elements. These constituents, even removed completely will still present in trace amounts starting from recovery till storage. They may have adverse effects such as causing corrosion and poisoning the catalysts. Nickel and vanadium along with iron and sodium are the major constituents of petroleum as metals. They can be determined by atomic absorption spectrometry and X-ray fluorescence spectroscopy.

- **Salt Content**

The salt content of the crude oil is highly dependent on their crude oil characteristics, and they are resulted principally from the production practices used in the field. Typically desalters are used to remove the salts from the crude oil. They are critical during crude oil processing since salts in small concentrations can accumulate in stills, heat exchangers, etc; leading to fouling and they require extensive cleanup. The evolved hydrochloric acid is extremely corrosive and in order to reduce its damage, ammonia is to be injected into the overhead lines to reduce corrosion. Thus the knowledge of salt content will help to find out whether and to what extent the crude oils need desalting.

- **Sulfur Content**

Sulfur is present in crude oil in the form of sulfides, mercaptans, thiophenes, benzothiophenes and dibenzothiophenes. Most of the cases, the sulfur is critical during processing because sulfur can act as a poison during catalysts. Typically they are present within the rough limits 0.1% w/w to 3.0% w/w. The formation of hydrogen sulfide along with different low boiling sulfur compounds are found during crude distillation. Hydrogen sulfide produces either from free hydrogen sulfide in the feedstocks or because of low temperature thermal decomposition of sulfur compounds.

- **Viscosity and Pour Point**

Viscosity and pour point characteristics are generally performed to check the flow characteristics of crude oil and its constituents at low temperatures. According to the thumb rule, it is said that lower the pour point of the crude oil, the more aromatic it is; and higher the pour point of the crude oil, the more paraffinic it is. The *viscosity index* is a widely measured property of the variation of kinematic viscosity due to the



changes in crude oil between 32 °C and 100 °C. For crude oils of similar kinematic viscosity, the higher the kinematic viscosity, the smaller is the effect of temperature on its kinematic viscosity. *Pour point* of petroleum is an index of the lowest temperature at which the crude oil will flow under specified conditions. Pour point data is used to supplement other measurements of cold flow behavior in different constituents, and these data is essential to find the wax properties of these constituents.

- **Water and Sediment**

Emphasis is given in reducing the content of water and sediment in crude oil during early processing as they may lead to difficulties in the refinery, for example - choking in heat exchangers, product quality effects, etc. Water along with different salts will act as an emulsion which can be easily removed. Knowledge of water and sediments is extremely important in accurately determining the volume of crude oil in sales and its economics. The sediments consists of finely divided solids that are typically drilling mud or sands or scale picked up during the transport of oil or may consists of chlorides obtained from brine. Sediments may lead to plugging of equipments and corrosion due to chloride decomposition.

- **Other Tests** Other properties which can be determined are Reid vapor pressure, total acid number and chlorine content. These quantities along with some other properties helps to build a petroleum assay and serves as a base for refinery linear programming.

# Chapter 7

## Refinery Planning Model in PIMS

### 7.1 Steps in creating a mathematical model

Before exploring the usage of mathematical tool Apen PIMS for making a refinery planning model, there are some intricate steps which are required for the modeling process. This steps will start from the present situation and will end with a fully optimized solution. The steps will be explained below :

#### 7.1.1 Problem Recognition

Problem recognition is one of the most important processes in modeling. This step is essential to identify what are the required steps which can be developed to improve the present situation. This step can also be used to identify the possible errors and hurdles which are going to take place prior in solving the problem and to use appropriate techniques for the improvement of the problem.

#### 7.1.2 Collect Information and Data

Once the problem is recognized and the model is approved, the job of the modeler is to collect information regarding the objectives of the model. These information need not to be well defined quantitative measures, but general statements of utility functions. Generally, the clients will not agree to a single objective function, so multi objective functions are preferred. It will be the responsibility of the modeler to quantify these utilities, determine proxy criteria and obtain some agreement regarding major shareholders and clients rearding the objective functions. The next step is the collection of data. This always takes more time than the first step as the data is often hard to come by due to the protective nature of the subordinate managers or other employees

who would guard their data as and when required. Other problems the modeler may face will be the unavailability of data.

### **7.1.3 Building The Model**

In particular, this step includes the definition of the variables, formulation of the objective functions and the constraints which are controlling the objective functions. While there are different ways to formulate a model and many ways to approach a problem, it is a good way to start the formulation of the model by the definition of variables. Sometimes there are so called logical variables too, which indicate whether an activity is carried out or not. These variables carry a value of one, only when we use them; else it will be zero. And there may be a lot more of these variables. So it is necessary to have a thorough understanding of each variables as each regular sentence will be translated into mathematical statement which will define a variable in the model.

### **7.1.4 Solving The Model**

This step is simple as different solvers will be used for the compilation of the model. Most famous solver is simplex method, primal method is another one which is used by PIMS.

### **7.1.5 Model Validation**

This important step will justify the examination of the solution obtained in the previous step. This step will help the modeler access the important questions of the errors in the model, the implementation of the solution regarding internal and external resistance from the organization will affect the solution? If the modeler is satisfied of the above questions, he can easily move to the next step which will be the implementation of the model. If not, he will go to the previous steps where he will make changes and try to converge the model.

### **7.1.6 Model Implementation**

This is the final step of the process. This involves the results of the model to be presented by the modeler to the appropriate decision makers and those who have the

power to approve it. In order to ensure the model to be put into practice, it is necessary that the results generated from the model should be consistent enough. In order to make the solutions 'sellable' to the decision makers, the solution is made optimal from one of the many possibilities to improve the situation, along with the detailed discussion of the assumptions taken which had led to the solution and the changes that have been resulted from the changes in the data.

## 7.2 Creating refinery planning model in PIMS

Refiners and petrochemical producers always face a challenge of competition, climate control policies, innovations and economics. The way to respond to these variables is by providing a solution with the most profitable operating plans, meeting necessary demands and making key changes which is compliant to the industrial standards and profit improvements. PIMS use linear programming to solve a wide variety of short term strategic planning problems, which are usually taking place in refineries and petrochemicals. The following are some of the key points which can be seen in the solution generated in PIMS.

### 7.2.1 The Solution

Aspen PIMS allows refining and petrochemical companies to develop optimal planning models which can be seen to balance the complexities of today's environment with maximum profitability.

- **Increased profits** through model accuracies. PIMS enables to model based on model analysis, crude and feedstock selection, production and operations planning and blending. It optimizes the model according to the data such as crude oil properties, crude fractionation and product specifications.
- **Reduced Operations Costs** through a detailed planning process which enables improved utilization of resources, right utility sizing and loss reduction.
- **Sustained Values** through common process models, consistent model validation and custom reporting of results.
- **Linear and Non-Linear Modeling**, especially Successive Linear Programming is a primary non linear feature. PIMS also provides non linear recursion, interaction blending, additive blending and mixed integer modeling.

- **Integration with spreadsheets and databases.** Interaction with PIMS is done using input and maintenance of model by the use of spreadsheets. Moreover, PIMS integrate Microsoft Access, SQL Server and Oracle with ease.
- **Windows Graphical User Interface** helps the user to adapt to the usability of the program. Model management, data management, matrix generation and solution all are easily accessible through the user interface.

### 7.2.2 Components of PIMS

PIMS consists of the following major components:

- **PIMS user interface** is used to view, modify and create various models. It also provides access to other basic components of PIMS.
- **Validation reporter** helps the user to check the consistency and liability of the model and helps to summarize the model.
- **Model documentor** is used to view and print the input data tables in the model.
- **Matrix Generator** is the most important part of the PIMS system. It gathers the data from the model and automatically converts it into the form of a linear programming model which represents the process economics, process technology and the material balance of the process. This is shown in a standard MPS format. It is also possible to generate a matrix generator report which will help the user to identify the matrix coefficients in the form of a column input.
- **LP Optimizer** in PIMS uses CPLEX or XPress. It reads the matrix from the matrix generator file, processes it (or optimizes it) and then return the results by giving an optimal solution. PIMS allows you to use the current solution of the file and use it as an input to that solution for future cases.
- **Solution Reporter** gathers the optimized solution and generates the summary and comprehensive reports. A summary report and a primal/dual solution report are created. It also develops a spreadsheet solution files to develop more custom reports.

## 7.3 The Structure of a Refinery Planning Model

Linear programming model of a refinery is intended to diaplay a wide assortment of events such as :

- Crude distillation
- Different processing units including catalytic crackers, hydrotreaters, hydrocrackers, reformers, desulfurizers and visbreakers
- Stream pooling
- Product quality recursion
- Blending of finished products
- Blending of refinery fuel
- Feedstocks for meeting product quality demands
- Exporting of different refinery streams to refineries

The refinery LP model, in fact, is simply a set of data tables in the form of spreadsheets that are converted into a matrix using special programming languages. As many solutions to the problem are possible, the criteria for choosing an optimum solution is that which, apart from satisfying all equations, gives maximum profit to the refinery. The optimum solution of a refinery LP model demonstrates the following:

- An entire, unitwise, feed and product values of all refinery units. The materials could be calculated in the basis of either weight or volume.
- The unit limits are made accessible and used.
- Feedstocks accessible and utilized for handling or blending
- Utilities (fuel, power, steam, cooling water), chemical composition and consumption of catalysts are essential for all handling units generally in a refinery.
- Composition of blending of feedstocks and products.
- A financial outline, which may incorporate the cost of crude oil, different feedstocks, utilities, chemicals and catalysts against the costs of finished products resulted from blending.

### **7.3.1 Rows and Columns Names and Types**

Rows and column names are given for simple identification and usage of information as and when required. In PIMS, the names of row and column will be seven characters in length. The initial four characters will distinguish the kind of the row or column, while the last three characters distinguish the stream. For example PURCXXX, SELLXXX, and so forth. Here XXX speaks to the name of the stream.

### 7.3.2 Units of the Row

The product of the units of a column and the units of a coefficient in a row consecutively measure up the units of a row. Therefore, if the column section points out a thousands tonnes in a day and a coefficient in the utility balance row adjust to 000' Btu/ton, the units of row are = 000' Tons/Day \* 000' Btu/Ton or million Btu/Day. Some of the technical limitations arises due to the following: feed availability; product demand; process yield; utility, catalyst, and chemical consumption; and product blend.

**Feed Availability** Feed availability equations mirrors the consumption of crude as well as the necessary feedstocks for further handling. The disposition of raw petroleum stock could be of various crude oils in various working modes. The usage of intermediate stock will be used for further downstream processing. For instance, if we are purchasing a crude named AVP having a specific volume of some value, it's vector will be denoted as PURCAVP and it will have the coefficient of -1. It's disposition in certain units will be denoted as SCRDA1N, SCRDA1K, etc which will have the coefficient of 1 indicating that the purchased crude will be utilized in these units.

**Product Demand** The demand of the product is embedded in the SELL table. The row names in this table are codes which are given to the product. These rows are generated in a matrix with a prefix VBAL showing their material balance relating to their demand to its blending. We can keep the request of the item as fixed, known as fixed grade product and the entry in the section is to be done in the column FIX in the sell table. In the event that the request of the item is not settled, it is called adjusting or free review, and it's generation is optimized, in light of the cost of the item, with most extreme or least request requirements if accessible.

**Process Yields** Different process units are ther in a refinery. Of which there are atmospheric residue and vacuum residue, which are obtained from the bottom part of the column. CDU downstream consists of other processing units, such as FCC, DCU, DHT, etc. There are different operating modes in a refinery. The operating mode is shown as a column in the unit submodel. The processing modes or feed names can be used as a column in the unit submodel. The rows are the result of the material adjust for every delivery. The yield of the product are shown in the product heading.

**Process Unit Capacities** Each unit has a capacity. This capacity is shown in the process capacity row. Each operating mode should have a row showing the capacity consumed for a particular unit of feed in a process unit. In a particular unit called SFCC as a submodel, the capacity row for that unit will be CCAPFCC and its coefficient will be 1. Likewise in table CAPS with process capacities, we can give a minimum (MIN) and maximum (MAX) limits for a particular model, lets say SFCC as CFCC.

**Product Blending** These conditions guarantee that the amount of streams delivered by process units are equivalent to the amount of blend stock accessible for mixing in addition to any material streams that going to refinery fuel. Likewise, the amount of blended stock utilized as a part of every item is made equivalent to the amount of completed item. By tradition, material or utility devoured by a procedure is appeared as positive and material delivered by a procedure is appeared as negative. For instance, if a unit devours 100 units of a crude, that is entered in the matrix as +100, though if this unrefined unit produces 20 units of crude naphtha, 25 units of kerosene, 30 units of diesel, and 25 units of refined naphtha, every one of these yields are entered in the matrix with a negative sign. Item mixing information are entered in the model as a table BLNMIX or as the properties of mix streams. The table BLNMIX is, indeed, a mixing map. The lines are the stream names and the section headings are the names of different item reviews. A section of 1 on the convergence of a line and segment demonstrates that the stream showed by line name is permitted to be mixed in the review demonstrated by the segment name. The absence of a section at this line/segment crossing point suggests that this mix stock is not permitted to be mixed in that review. Blend stream properties originating from the crude and vacuum refining units are entered in an ASSAYS table. The properties of process unit streams are entered in various tables called mix properties, or BLNPROP. In the event that pooling various streams shapes a stream, its properties are obscure. Be that as it may, an underlying theory of its properties is required to begin the enhancement procedure. Such speculated information are likewise given in PGUESS table.

### 7.3.3 Property from other subtables

In PIMS, the properties of straightrun streams are either taken from ASSAYS or BLNPROP. These properties, need not to be re-entered, instead placeholders (999) are put in, which the data will be replaced from the relevant data table. By tradition, a negative sign is utilized for streams entering a recursed pool and their properties



and a positive sign for the pool created. Placeholder determination can happen in client characterized E-, L-, or G-sort pushes and in addition in recursion columns. Placeholders for recursed properties are supplanted by the most recent estimation of the recursed property of a stream each time the matrix is refreshed.

### **7.3.4 Blending Specifications**

These equations ensure that each optimal product blends meet the required specifications set for it. The entries of different blending streams will be given in the table BLNSPEC.

### **7.3.5 Stream Pooling**

It is often seen that more than one streams will be acting as a feed in a particular unit. For dealing with these kind of streams, it is often advisable to include those streams as a pool and create a feed pooler. The client must supply information on the properties of the pooled stream for streamlining agent to achieve an answer. The client, in any case, has an issue, on the grounds that the creation of the pooled stream is not known until after the ideal arrangement is come to. An iterative approach (recursion) is utilized. The client gives a first figure on the properties of pooled stream. The streamlining agent then explains the model with the evaluated information in it. In the wake of illuminating the model, an outer program recalculates the physical properties of the pooled stream, which was prior speculated. The changed physical property information are embedded in the model, and the model is run once more. The cycle proceeds until the delta between the information and yield properties of the pooled stream are inside determined resilience limits. Recursion is, accordingly, a procedure of comprehending a model, inspecting the ideal arrangement, utilizing an outside program, ascertaining the physical property information, refreshing the model utilizing the computed information, and illuminating the model once more. This procedure is rehashed until the adjustments in the figured information are inside the predetermined resilience. By tradition, the streams entering the pool will have a negative sign and the streams leaving the pool will have a positive sign. The name of this column will be RBALXXX, where XXX is the pool tag.

The following couple of columns will have names beginning with RYYYXXX, where YYY will be a property which is to be recursed, while XXX will be the tag of the stream. It is easy to realize that the properties of the pooled stream will not be

available at first; thusly to discover them, a figure is given in a different table PGUESS. The model is next keep running with these pool properties and the pool properties recalculated, in view of new exercises of the vectors. In the event that the recalculated pool properties are unaltered or inside the resistance a cutoff of the prior qualities, the recursion procedure is halted and the arrangement is said to have met.

### 7.3.6 Distributed Recursion

Before explaining about distributive recursion, it is essential to shed some light in recursion. *Recursion* is the process of solving a model, examining the optimum solution using an external program, calculating physical property data, updating the model using the calculated data, and solving the model again. This process is repeated until the changes in the calculated data are within specified tolerances.

In the early days of linear programming, when a model was built to represent a process such as a refinery, there was, of necessity, data in the model that had to be estimated. This data was usually physical property data of materials used in the refinery to produce refined products. For example, gasoline is blended in a refinery to meet certain specifications for octane, vapor pressure, sulfur content, distillation, etc. Therefore, when blending data was provided for each of the blend components to be used by the optimizer to blend gasoline, the user estimated most of this data. Unfortunately, much of this data were dependent on other factors such as feedstock qualities and operating conditions. In other words, they were dependent on the composition of the crude slate feeding the refinery or the way the refinery process units were operated. The cut point for each material coming from the crude unit was a factor, as well as the severity at which the reformer was run and the ratio of C3 olefin to C4 olefin in the feed to the alkylation unit.

Because much of this data were estimated or guessed at by the user, the data in the model was inaccurate or wrong. To compensate for this, a technique was developed to improve the data as the model was being solved. This technique, which came to be known as recursion, was very ingenious. The optimizer first solved the model with the estimated data in it. After solving the model, an external computer program written in a computer language such as, Fortran, PL/1, or Assembly Language, calculated the physical property data being used in the model from the optimum solution. In other words, the external program examined the optimum solution just produced by the optimizer and calculated the physical property data of the crude fractions by using the composition of the crude slate in the solution. This data was then inserted into the

model (LP matrix) thereby updating the estimated data with more accurate data. The model was resubmitted to the optimizer and solved again. The same external program then examined this second solution, the same data recalculated, the recalculated data inserted into the matrix and model is solved again. This process was repeated until the changes taking place in the calculated data were small enough to be within certain tolerances specified in the external program.

In the basic recursion handle, the contrast between the client's figure and the ideal explained esteem is computed in an outer program, refreshed, and settled. The *distributive recursion* show moves the error estimation method from outside the direct program to the LP grid itself. With this game plan, the ideal that is come to has the physical property information for all recurred streams precisely coordinating the organization of the pool used to make those properties. After the present framework is understood, utilizing the underlying physical property gauges or speculations, the new values are processed and embedded into the matrix for another LP arrangement. The significant distinction between distributive recursion and ordinary recursion is the treatment of the contrast between the genuine arrangement and the figure. This distinction is alluded to as a error. At the point when a client surmises the recurred property of a pooled stream, the "error" is made in light of the fact that the client figure is constantly wrong. The distributive piece of the distributive recursion is that this mistake is conveyed to where the quality is being utilized. A pooled stream can go to various item reviews or progress toward becoming food to a procedure unit. The error vector is disseminated wherever the pooled stream property is utilized. As it were, one might say that the pooled stream properties are spoken to by two vectors, one is the underlying speculation of the property and the second is the mistake or redress vector that tries to align the property with property registered from the structure of the mix.

### **7.3.7 Objective Function**

To run the procedure of optimization, an additional line, called the objective function, is required. The optimization procedure either limits or boosts this capacity, contingent upon whether the capacity speaks to the refinery working expense or benefit. All cost vectors must have a section in the target work push. The coefficients in this line are the expenses per unit of item delivered. The cost of crude and different encourages, for example, flammable gas, or utilities are entered with a negative coefficient if the target work speaks to general benefit to the refinery.

### 7.3.8 Interpretation of the Solution Report

The output of the model will be a sort of an improper report, with a listing of rows and columns as same as the output.

**Rows** : The yield for each row gives the name of the row provided by the user.

**BS:** 'Basis' means that the row is not restricted to upper and lower bound.

**LL:** 'Lower Limit' means that the final solution is restricted at a lower level by a lower bound given in this row.

**UL:** 'Upper Limit' means that the last solution is limited to the upper level by an upper bound given in this row.

**EQ:** 'Equal' means that the last solution is bounded to the fixed right hand side. This means the upper and lower bounds are equal.

**Columns** Each output of the column shows the Column name. The names of the column are normally generated by the application or given by the user as the input for the tables for generation of the matrix.

**Activity:** This is the estimation of a variable in the last solution. A few factors in the basis may have no action by any stretch at all. Factors with zero action might be in the basis on the grounds that a specific number of factors (equivalent to the quantity of rows) are required to be in the basis by the way of LP strategy. Input costs. These are the coefficients found in the row of the objective function, and they enable aggregate cost and incomes to be represented in the row of the objective function.

**Lower limit:** This is as far as possible (called bring down bound) that estimation of an activity can have..

**Upper limit:** This is as far as possible (called upper bound) that estimation of an activity can have.

**Reduced cost:** This is otherwise called the D-J or Delta-J value. It is a result of reduction in net benefit or increment in least cost, if a movement, not in the premise, is brought into the premise and given the estimation of 1. This is cost of utilizing an activity that is not some portion of ideal arrangement. Every diminished cost are zero or positive in a solution which is deemed to be optimal.

### **7.3.9 Delta Modeling**

Delta-based modeling (DBM) is a method used to foresee the yields and properties of the procedure units, when the yields and the properties are a component of the sustain quality. As a rule, the nourish is a pool of streams whose synthesis must be controlled by the advancement procedure itself. Delta-based displaying is helpful in these circumstances when consolidated with distributive recursion methods. To execute the DBM, an encourage quality parameter is characterized that can be measured effortlessly and identified with the yield of the unit. For instance, the yield of reformat is known to be an element of naphthene in addition to twice aromatic ( $N + 2A$ ) substance of the feed. Assume the base case reformer yields are characterized for an feed with a ( $N + 2A$ ) substance of 30. In most LP applications, the feed is assumed to be a pool of streams whose piece must be controlled by the optimization. In this way, the properties of the feed to the unit are obscure. Subsequent to pooling different catalytic reformer feed streams, if the model processes the feed to the reformer at ( $N + 2A$ ) content at 45, a yield error correction vector redresses the base respects relate to a sustain with a ( $N + 2A$ ) value of 45.

## **7.4 Crude Distillation Modeling**

LP models for crude and vacuum refining can be developed precisely in an indistinguishable way from done on account of different process unit submodels. Most refineries may have more than one crude unit and might prepare more than one unrefined petroleum. Likewise, an unrefined unit may work in more than one mode; for instance, one crude unit mode may expand the generation of naphtha and another may amplify the creation of diesel. It is, thusly, helpful to enter all information on yields and properties of the different cuts from various unrefined oils and crude and vacuum refining units display and their utility utilization, pooling of different cuts from crude and vacuum units in three tables for simple updating of data.

### **7.4.1 ASSAYS**

Information as yields of different unrefined on various CDUs and properties of cut delivered is entered in a solitary table, the Assay Table (ASSAYS). This table does not specifically create any matrix but rather just gives information to crude and vacuum

units demonstrating. The yields in the Assay Table could be either in volume or weight units. The section names in the table are three character operation modes<sup>5</sup> of different unrefined segments. There are four sorts of lines in this table. The primary arrangement of columns is utilized to give cut yields. The line names are VBALXXX, WBALXXX, or DBALXXX. VBAL and WBAL demonstrate a volume or weight based yield. The label XXX is the name of the cut created from the refining. The DBAL push characterizes a cut being delivered not on the unrefined refining unit but rather from a downstream unit. For instance, a crude refining section may create a wide cut containing naphtha and some kerosene in a downstream naphtha fractionation section. For this situation, as naphtha is not being really delivered on the unrefined section but rather elsewhere, it will be spoken to in the ASSAY Table by the DBAL row rather than the VBAL row. The second arrangement of lines might be utilized to indicate atmospheric or vacuum unit utility utilization that is unrefined particular. The line name for this set is as UATMxxx or UVACxxx, where xxx is the utility devoured. A third arrangement of columns might be utilized to indicate atmospheric or vacuum unit limit utilization values that are unrefined particular. The line name for this set is CCAPATM or CCAPVAC, and the sections for every crude are the units of limit expended per unit charged to the air and vacuum towers. The fourth arrangement of columns is utilized to give cut properties. The column names for this set are Ipppxxx where ppp is the property (SPG, SUL, API, and so forth.) and XXX is the cut name. The primary letter, I, shows this is property information. The second through fourth characters of the line name recognize the property, while the last three characters distinguish the procedure stream to which this property applies: ISPGLN1 Specific gravity of LN1. ISULLN1 Sulfur substance of cut LN1. IVIILN1 Viscosity mix file of cut LN1. The coefficients in the I lines are the estimations of the particular property of a predetermined stream. I rows will not be displayed in the matrix. The LP display utilizes this information by duplicating, for instance, ISPGLN1, with volumes in column VBALLN1 and setting the outcome in recursion push RSPGLN1 for processing the particular gravity of a mix of streams.

## 7.4.2 CRDDISTL

This table is utilized by the model to characterize the structure of various hypothetical or legitimate crude refining submodels. Each logical crude unit might be viewed as one of numerous methods of operation of a crude unit. This table gives mapping between the ASSAYS Table information and these legitimate unrefined units. The

* TABLE	CRDDISTL	
*	Crude Distillation Map	CDU-1
	TEXT	CD1
*		
*	Atm & Vac Tower Map:	
ATMTWR	Physical Atm Tower	1
VACTWR	Physical Vac Tower	1
*		
*	Estimated Crude Charge:	
*	Sweet Crude Mix:	
ESTABC	CRUDE ABC	40
ESTDEF	CRUDE PQR	60
*	Sour Crude Mix:	
ESTPQR	CRUDE PQR	20
ESTXYZ	CRUDE XYZ	80
*		
*	Utilities (per Ton):	
ATMFUL	Atm Twr FUL	0.3
ATMKWH	Atm Twr KWH, KWH	5.7
ATMSTM	Atm Twr STM, MT	0.0458
*		
VACFUL	Vac Twr FUL	0.024
VACKWH	Vac Twr KWH, KWH	4.19
VACSTM	Vac Twr STM, MT	0.143

Fig. 7.1  
TABLE CRDDISTL

segment names are three character labels for different operation methods of a crude units. Where singular crudes are being isolated, it might be helpful to utilize crude tags as legitimate unit labels, however this is not a necessity. The lines of this table are isolated into four sets. The main set includes row names ATMTWR and VACTWR. The passages in these columns are number qualities demonstrating which physical crude refining towers are utilized by different coherent unrefined units. The second arrangement of columns are ESTXXX, where XXX is the crude tag. The sections in these lines characterize the assessed charge of every unrefined to each logical crude unit. These evaluations require not be precise. The charge assessments are either on a weight or volume basis, contingent upon how crude measure information are entered. Along these lines, if the unrefined measure information are on a volume premise, passages in this table ought to be in volume units. The LP display utilizes these information to ascertain the properties of straight-run cuts from a predefined crude blend. The following arrangement of lines in this table are named ATMUUU and VACUUU and these characterize the utilization of utilities (fuel, steam, power, cooling water, and so forth) in atmospheric and vacuum units for each of logical crude units.

### 7.4.3 CRDCUTS

The CRDCUTS Table characterizes the unrefined refining cutting plan utilized as a part of the model. The column names are the three-character stream labels of the straight-run refining cuts. The segment TYPE is utilized to distinguish the sort of cut, and each cut must be assigned one of the accompanying numbers: Generally the seller provided LP bundles have an in-manufactured system to create an Atmospheric Distillation Unit sub model. Different types of cuts are as follows:

- **0** This demonstrates cut yield is recognized in the assay information, however this cut is delivered by downstream partition, in a saturated gas plant and not on a crude unit.
- **1** This shows this a straight-run atmospheric cut.
- **2** This shows it is atmospheric residuum, which might be utilized somewhere else or fractionated in a vacuum unit. On the off chance that an atmospheric residue is constantly coordinated to a vacuum unit, it is overlooked from the cutting scheme in this table.
- **3** This shows it is a straight-run vacuum cut.



*TABLE	CRDCUTS		
*	CRUDE CUT DETAILS		
*	CRUDE TYPE		SWEET
ROWNAMES	TEXT	TYPE	CD1
FGG	CDU FUEL GAS	1	1
VLP	CDU LPG	1	1
LN1	CDU LN	1	1
MN1	CDU MN	1	1
HN1	CDU HN	1	1
SH1	CDU SIDECUT HN	1	1
KR1	CDU KERO	1	1
KS1	CDU KERO ST RUN	1	1
CL1	CDU LGO	1	1
CH1	CDU HGO	1	1
VL1	CDU LVGO	3	1
VH1	CDU HVGO	3	1
VS1	CDU VACSLOP	3	1
VR1	CDU VR	3	1
LOS	LOSS	3	1

Fig. 7.2  
TABLE CRDCUTS

- 9 This demonstrates it is a deferred cut that is not created on a crude refining unit but rather in a downstream unit.

The other column names in this table are the three-character labels for the logical crude units and should precisely coordinate the segment names of the CRDDISTL Table. The section at every crossing point is the pool number to which the cut from each coherent crude unit is coordinated. For instance, if this table contains a cut ABC, this stream yields streams AB1 in pool 1, AB2 in pool 2, and AB3 in pool 3. In this way, when a stream is isolated, the model consequently develops extra stream labels to recognize the isolated stream. The third character in the stream tag is supplanted with a pool number for pool 2 forward.

#### 7.4.4 SCR D

*TABLE	SCR D											
*	CRUDE DISPOSITION SUMMARY											
ROWNAMES	TEXT	A1N	A1K	A2N	A2K	A3N	A3K	A4N	A4K	A5N	A5K	
VBALABC	CRUDE ABC	1	1	1	1	1	1	1	1	1	1	1
VBALA1N	ABC TO CDU1 NORMAL MODE	-1										
VBALA1K	ABC TO CDU1 KERO MODE		-1									
VBALA2N	ABC TO CDU2 NORMAL MODE			-1								
VBALA2K	ABC TO CDU2 KERO MODE				-1							
VBALA3N	ABC TO CDU3 NORMAL MODE					-1						
VBALA3K	ABC TO CDU3 KERO MODE						-1					
VBALA4N	ABC TO CDU4 NORMAL MODE							-1				
VBALA4K	ABC TO CDU4 KERO MODE								-1			
VBALA5N	ABC TO CDU5 NORMAL MODE									-1		
VBALA5K	ABC TO CDU5 KERO MODE										-1	

Fig. 7.3  
TABLE SCR D

The SCR D table demonstrates the disposition of the crude obtained and prepared by the refinery to different crude refining units. Just those crudes with nonblank entries in the material adjust columns for crudes are accessible as a potential feed to the logical crude unit. In this manner, if a crude is excluded in that unit, it won't be handled in that specific unit. The essential cuts from different crude units are pooled according to pooling map in the CRDCUTS Table. Consequently, all refinery climatic refining information is kept up in these tables. The CDU models are naturally created from them by the LP bundle.

## 7.5 Vacuum Distillation Modeling

In refineries in which each CDU has its own related VDU, modeling a composite crude and vacuum unit turns out to be simple, and yields from the vacuum unit are dealt with precisely like those from CDU. Notwithstanding, in refineries where atmospheric residuum from a given CDU can go to various VDUs, one can't regard CDUs and VDUs as a solitary mix, since one doesn't know ahead of time in which VDU a given atmospheric residue will be handled nor which set of vacuum streams will be created. The benefit of modeling vacuum refining with deferred cuts and the stream's pseudo properties are as per the following:

1. The count of all VDU yields and stream properties are done in the Assay Table and transmitted to the particular VDU demonstrate. The VDU models themselves contain no yield information. All information upkeep is just through the Assays Table.
2. Just a single environmental resid stream is created for each CDU, regardless of the quantity of crudes prepared in it. Without conceded refining, one atmosphere residue is produced for each crude.
3. For every VDU, just a single arrangement of vacuum streams is created, as opposed to a different set for every unrefined/CDU/VDU mix.
4. The streams delivered in the model compare a great deal more intently to streams physically created in the refinery.
5. All vacuum yields are determined in the Assays Table, disposing of the need to keep up vacuum yield information in VDU submodels.

# Chapter 8

## Results and Discussion

As per the discussion in Auto Fuel Vision and Policy (2014), it has been made mandatory for the administration to produce 100% BS VI fuels from 2020. Moreover the reduction of sulfur in auto fuel, especially in diesel, gives a much open conditions for emission control by treating them. As it is known that sulfur exists in gasoline and diesel in the form of aromatic compounds ranging from mercaptans, thiophenes, benzothiophenes, di-benzothiophenes, etc. As the refiners are forced to produce fuels with lower allowable 'sulfur', the refiners are challenged themselves to research about different variations of hydro-desulfurization process. The process of removing these compounds from fuels are kinetically limited, which makes it difficult to plan and establish such expensive units.

With reducing sulfur in fuels by 10 ppm, there would be a lower particulate matter load and the  $NO_x$  device will also benefit from lesser  $SO_x$  in the exhaust and thus lesser catalyst deactivation rates. It can be said that emission control systems will be benefited with less sulfur content fuel. But on the other side, if the sulfur levels are reduced, fuel stability is affected as reduced thermal stability will lead to issues like fuel filter plugging. These are some of the problems which should be addressed by the refiner.

So the refiners are compelled to evaluate options for new process units as well as upgradation of existing process units to comply with these specifications.

### 8.1 Objective

The primary objective of the study is to evaluate options to produce MS and diesel conforming to BS-VI specifications. The current refinery configuration was modeled to produce BS VI quality MS and Diesel.

Table 8.1 Specification of BS-VI MS Regular and Premium

Sr No.	Attribute	Unit	BS-VI MS Regular	BS-VI MS Premium
1	Density at 15°C	kg/m <sup>3</sup>	720-775	720-775
2	Distillation			
	E-70	% vol	10-40	10-40
	E-100	% vol	40-70	40-70
	E-150	% vol, min	75	75
	FBP	°C, max	210	210
3	Sulfur	wppm, max	10	10
4	RON	min.	91	95
	MON	min.	81	85
5	RVP at 38 °C	kPa	60	60
6	Benzene	% vol, max	1	1
7	Aromatics	% vol, max	35	35
8	Olefins	% vol, max	21	18

Table 8.2 Specifications of BS-VI Diesel

Sr No.	Attribute	Unit	BS-VI Diesel
1	Density at 15°C	kg/m <sup>3</sup>	820-860
2	Distillation T95	°C, max	370
3	Sulfur	wppm max	10
4	Cetane number	min.	51
5	Cetane index	min.	46
6	Flash point	°C, min	35
7	Viscosity at 40 °C	cSt	2.0-4.5

## **8.2 Refinery Configuration : LP Modeling Development**

It is found clearly according to the speculations above that the main shift is indeed with respect to sulfur. In both gasoline and diesel, the sulfur specifications has been reduced to 10 ppmw levels. On analyzing the Gasoline and Diesel pools of the refinery, following observations were made:

### **8.2.1 BS IV Compilant Diesel Hydrotreating Unit**

The refinery consists of Diesel Hydrotreating Unit producing Diesel conforming to BS IV specifications, i.e. 50 ppmw sulfur. The majority of diesel pool is comprised of these streams. In order to achieve BS VI specifications of Diesel, it was decided that the catalyst change in DHT should be done. The latest generation catalysts with improved desulfurization properties makes it possible to achieve the desired results under slightly severe conditions in the unit.

### **8.2.2 BS IV Compilant VGO Hydrotreating Unit**

The refinery was planned to process VGO in a hydrotreater. The main product of these units is hydrotreated diesel conforming to BS IV specifications. Similar catalyst changes were envisaged in these units for producing diesel conforming to BS VI specifications.

### **8.2.3 Fluidized Catalytic Cracking Unit**

It was observed that for MS pool, the main sulfur contribution is from Gasoline produced in Fluidized Catalytic Cracking Unit. The mercaptans are found to be as much as 125 ppm typically in the light gasoline from fluid catalytic cracking unit and it is essential to reduce to about 5 ppm before this stock can be used for blending in gasoline grades. One way of achieving this feat is by bringing it directly into the Merox reactor from the bottom of the FCCU debutanizer column. More about this can be found in the literature about Light Gasoline Merox Treating.

Another way of reducing the sulfur in FCC gasoline is by introducing noble metals as catalysts. For example, (Myrstad et al. 2002) explained a composition consisting of hydrotalcite material impregnated with metal additive such as Zn, called as Lewis

Feed/Product	Base Case	FCC Gasoline Treatment Unit	VGO Hydrotreater Unit
Crude	15.0	15.0	15.0
Fuel Oil Import	509	474	481
RLNG	454	313	337
Poly Propylene	407	410	386
LPG	852	835	781
Naphtha	916	1100	1011
MS BS IV	1229	0	0
MS BS VI	0	1200	1250
ATF	X	X	X
Kerosene	X	X	X
HSD BS VI	5233	5233	5233
Heavy Distillates	3345	3242	3041

Acid; the impregnated hydrotalcite material can be impregnated into the FCC catalyst as well as they can be used as a separate compound next to FCC catalyst. He found that additives with Ti and Zn showed the best performance (Zhao et al. 2001). Typically, different sulfur species present in FCC gasoline can be categorized into four groups:

- Saturates
- Thiophene (Th) + C1-thiophene
- C2-C4 thiophenes (ethyl-butyl thiophene)
- Benzothiophene

Mercaptans, sulfides, disulfides and tetrahydrothiophene comprise the group of saturates. C2–C4 thiophenes and benzothiophene comprise a major portion of FCC gasoline sulfur. Th and C1-Th are present in lower amounts. The probable reaction sequence for reduction of sulfur includes the following steps:

- Dealkylation of C2–C4 thiophenes to thiophenes + C1 thiophenes;
- Saturation of thiophene + C1 thiophene;
- Cracking to  $H_2S$ .

However, the following two major cases were studied:

- A Option with FCC Gasoline Treatment Unit
- B Option with VGO Hydrotreater Unit

In the above table, X means the value is same as the base case.

Some of the inferences made are :

- The VGO-HDT option was having higher margins in terms of GRM than that of FCC Gasoline Treatment units.
- The capacity of VGO-HDT was roughly about 2.0 MMTPA and that of FCC Gasoline treatment unit was about 0.6 MMTPA.
- Unit Capex were estimated based on past jobs for the above mentioned capacities and the payback period was estimated.
- The payback period of FCC Gasoline treatment option was more attractive than that of VGO-HDT option despite VGO-HDT option having more GRM. This is because of the fact that VGO-HDT being high pressure unit and of higher capacity, the Capex was more in that case. Also having post treatment unit gives much more flexibility to the refiner in terms of processing FCC feeds.
- Based on above advantages, an FCC gasoline treatment unit was recommended to meet the BS VI gasoline specifications.

The above points makes it clear that the Base case design with FCCU is a feasible option as compared to the Base case design with VGO HDT as the Capex was more in the latter.

### **8.3 Conclusion**

It was evident from the results that establishing a VGO HDT was not a feasible option. This project was closed by performing the detailed utility consumption studies, Capex and financial analysis. The utility consumption and pricing of the feedstock purchases and blended products are not included in this report for confidentiality purposes.





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