Planning & Optimization for an Oil Refinery with NO_X Reduction

BY

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A Thesis Presented to the
DEANSHIP OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

In

CHEMICAL ENGINEERING

JUNE 2011

KING FAHD UNIVERSITY OF PETROLEUM AND MINERALS
DHAHRAN, SAUDI ARABIA
DEANSHIP OF GRADUATE STUDIES

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Dedicated

To My Family

Acknowledgement

All praise be to Allah, Lord of the worlds, the Almighty, with whose gracious help it was possible to accomplish this task. Acknowledgement is due to King Fahd University of Petroleum and Minerals (KFUPM) for supporting this thesis report. Without their support, this work would not have been accomplished.

I would like to express my appreciation to my advisor Dr.Mohammed Ba-Shammakh for his help, guidance and attention that he devoted throughout the course of this work. Special thanks are also due to the thesis committee members Dr. Housam Binous, Dr. Naim M. Faqir, Dr. Eid M. Al-Mutairi and Dr. Abdullah Al-Shammari for their cooperation and constructive advice.

Special thanks are also due to the chairman of Chemical Engineering Department Dr. Usamah A. Al-Mubaiyedh, for his moral support and good wishes, and all my department colleagues for the memorable days shared together.

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Abstract (English)

Name: Fayez Nasir Al-Rowaili

Title: Planning & Optimization for an Oil Refinery with NOx Reduction.

Degree: MASTER OF SCIENCE

Major Field: CHEMICAL ENGINEERING

Date of Degree: June 2011

Today science is concerned with toxic emissions from refineries, such as NO_X. This research work is concerned with studying NO_X emission from oil refineries. When NO_X exists in large amounts, it could cause different types of serious diseases and illnesses like lung and breathing problems to human being and animals. Due to the dangerous effects of NO_X on the environment and human health, it becomes essential for science to do deep research in this area, in order to find optimal ways of NO_X reduction. The purpose of the study is to find how to reduce NO_X emissions from oil refineries using different methods while maintaining profits at the maximum possible value. The three methods being used for NO_X reduction are; balancing, fuel switching and use of technology for NO_X reduction. I will try to reduce NO_X emissions using the above three methods with different reduction percentage ranging from 20% to 80%. The profits of the oil refinery for each reduction target of NO_X will be analyzed and looked at closely. As it should be stated in this research work, my goal is to find the optimal profits considering the required NO_X reduction percentage through the use of the GAMS software General Algebraic Management System. GAMS will assist in calculating total cost and profits for different cases with different NO_X reduction percentages. GAMS, in addition to giving profits values can tell us, among the three NO_X reduction methods, which method will be used for each unit of the oil refinery in order to keep the profits at the maximum possible value.

Key Words: Planning in Oil Refinery, Optimization, NO_x Reduction Technology

MASTER OF SCIENCE DEGREE

KING FAHD UNIVERSITY OF PETROLEUM AND MINERALS

JUNE 2011

Abstract (Arabic)

خلاصة الإطروحة

الاسم : فايز ناصر صليبي الرويلي

العنوان : التخطيط والتوخي الأمثل في معمل تكرير الزيت مع تقليل انبعاثات الــ NO_x (أكاسيد النتروجين)

الشهادة : ماجستير علوم

التخصص : هندسة كيميائية

تاريخ الشهادة.: يونيو 2011

إن العلم مهتم اليوم بالإنبعاثات السامة من المصانع وعلي سبيل المثال، الــ NO_x أو اكاسيد النيتروجين السامة هذا البحث معنى بدراسة انبعثات الـ NO_x بكميات كبيرة قد تتسبب في كثير من الأمراض: كأمراض الرئة والجهاز التنفسي . ويسبب التأثيرات السلبية لـ NO_x على البيئة والصحة الإنسانية . أصبح من الضروري أن يتجه العلم بشكل أعمق في هذه الناحية البحثية . إن الهدف من هذا البحث هو أيجاد الكيفية لتقليل إنبعاثات الــ NO_x من المعمل بعدة طرق وفي نفس الوقت محاولة الحصول على أقصى ربح ممكن إن الطرق العلمية المطروحة في البحث لتقليل الـ NO_x هي : التوازن بين الوحدات المعملية في الوقود المستخدم وتغيير الوقود المستخدم لنوع آخر من الوقود واستخدام تقنية حديثة لتقليل الــ NO_x . سأقوم في هذا البحث باستخدام هذه الطرق الثلاث لتقليل إنبعاثات الـ NO_x من معمل تكرير الزيت بنسب مختلفة تتراوح من 20 % إلي 80 % . سأقوم في هذا البحث بحساب الأرباح الصافية للمعمل لكل نسبة تقليل مقترحة لإنبعاثات الــ NO_x . أن هدفي في البحث هو إيجاد الأرباح المثلي للمعمل من خلال استعمال برنامج الـ GAMS لتحليل البيانات والحصول على القيمة المثلى للأرباح الصافية . الـ GAMS سيقوم بحساب الأرباح عند نسب مختلفة لـ NO_x ، بالإضافة لمعرفة الأرباح . فإن برنامج الـGAMS يقترح علينا أفضل طريقة من الطرق الثلاث المذكورة لتقليل الــ إنبعاثات NO_x في كل وحدة من وحدات المعمل .

درجة الماجستير في العلوم
جامعة الملك فهد للبترول والمعادن يونيو 2011

Chapter 1

Introduction

Petroleum is a complex mixture of many compounds of organic liquids called crude oil and natural gas. These organic liquids occur naturally in the ground and they formed millions of years ago. Crude oil is not the same everywhere but it varies from one location to another location in color and composition. It varies in color from a pale yellow low viscosity liquid to heavy black ‘treacle’ consistency. Crude oil and natural gas are extracted from the ground, on land or under the oceans, by drilling an oil well. Then, oil is transported by pipeline and/or ship to refineries where their components are processed into refined products. Crude oil and natural gas are of little use in their raw state. However, their value lies in what is created from them: fuels, lubricating oils, waxes asphalt, petrochemicals and pipeline quality natural gas. An oil refinery is an organized and coordinated arrangement of manufacturing processes designed to produce physical and chemical changes in crude oil to convert it into everyday products like petrol diesel, lubricating oil, fuel and bitumen. Crude oil coming from wells contains mixture of hydrocarbon compounds and relatively small quantities of other materials such as sulphur, oxygen, nitrogen, salt and water. Most of these non-hydrocarbon substances are removed in the oil refinery processes where the oil is broken down into its various components, and blended into useful products. The crude contains hundreds of compounds which vary in their properties and composition. A series of complex processes are required in order to convert the complex of hydrocarbons mixture into lighter compounds like gasoline and gas oil or diesel. The conversion process is the main task for an oil refinery.

A petroleum refinery is an extremely complex plant. However, in order to maximize profits from refinery, it requires that refinery operations optimize streams flow and process feed. Refining processes are central key components and a crucial link in oil supply chain. It is where crude petroleum is transformed into products that can be used as transportation and industrial fuels and for the manufacture of plastics, fibers, synthetic rubbers and many other useful commercial products. In general, an oil refinery is made up of several different parts. Various processing units that separate crude oil into different fractions or cuts, upgrade and purify some of these cuts, and convert heavy fractions to light, more useful, fractions. Utility systems are referring for the systems and process that provide the refinery with fuel, flaring capability, electricity, steam , cooling water, effluent treatment, fire water, sweet water, compressed air, nitrogen, etc., all of which are necessary for a refinery operation. Tank farm is where all crude, finished products and intermediates are stored prior to usage or disposal. Tank farms are the facilities for receipt of crude oil and blending and dispatch of finished products.

A modern oil refinery processes crude oil into high value products at minimal cost with minimal environmental burden. Refineries produce a wide range of petroleum products, including gasoline, diesel, heating oil, residual fuel, cock, lubricants asphalt, and waxes, as well non hydrocarbon products such as sulfur and vanadium. Petroleum products are used in many areas of our lives: gasoline to run cars, heating oil to warm houses, asphalt to pave roads, as well as other petroleum-based products such as plastics, medicine, etc. .

The critical objective of a refinery operation, as in any other business-oriented ventures, is to generate maximum profit by converting crude oils into valuable products. Expectedly, there are many decisions to be considered to achieve an optimal operation for a refinery. At the planning level, the need to decide the types of crude oil(s) to process, the types of products to produce, the operating route to use, the best operating mode for each process, the type of catalyst to select for each process, and others. At the process level, there is a necessity to determine detailed operating conditions. Namely, temperatures, pressures, detailed process flows, and other values of processing variables. All these decisions interact with another; for example, a temperature change in a reactor would result in different product yields and distribution, and also utility consumption, hence a different process performance would result. These are bound to implicate and affect the decisions made at the planning level to select raw material feeds for the process involved and even possibly influence the overall operating scheme. Consequently, integration of refinery optimization for short is considered one of the most difficult and challenging applications of large-scale optimization but the expected outcome would be commensurable with the effort, time, and resources invested.

The chemical process industry has been increasingly pursuing the use of computing technology to gather, organize, disseminate, and exploit enterprise information and to closely coordinate the decisions made at various levels of the process operational hierarchy so as to optimize overall corporate objectives. In refinery management, computer software is commonly deployed to assist in terms of planning, scheduling, and control functions by executing effective decisions chiefly pertaining to crude oil selection, production planning, inventory control, and logistics of transport and dispatch management. Continuous research and development in these aspects have gained practical significance, as observed. In this respect, we support the notion advanced by Li, Zhange and Zhu , Bassett et al and Bodington, that the preferred approach for achieving integration of planning and operations functions is through the formulation and solution of suitably structured mathematical programming models as they have been proven to offer the most effective tools. Indeed, it is the governing theme of this work that mathematical optimization offer the most effective framework for the integration at the strategic, tactical, and operational levels of refineries. This shall provide the thrust for undertaking the current work in this thesis research with ultimate objective of developing better management tools for decision-makers. In particular, this work considers the mathematical programming approaches for modeling the problem parameters for the planning of an oil refinery. Moreover, we should consider constraints like NO_X, SO_X & CO_2 reduction regulations which are enforced into the refinery. This is why optimization model builders should consider the air pollutants into their models.

Air pollutants produced by refineries are very risky to human health. In addition air pollutants can damage on the ozone layer, water and air. Table 1.1 below shows some of the major air pollutants emitted by refineries.

Table 1.1: Air Pollutants Produced by Oil Refinery

Main Air Pollutants	**Main Sources**
CO_2	Process fumaces, broilers, gas turbines. Fluidized catalytic cracking regenerators, CO broilers, Flare systems, and Incinerators.
SO_x	Process fumaces, broilers, gas turbines. Fluidized catalytic cracking regenerators, CO broilers, Coke calciners, Sulphur recovery unit (SRU)
NO_x	Process fumaces, broilers, gas turbines. Fluidized catalytic cracking regenerator, Coke calciners, Flare systems, and Incinerators.
CO	Process furnaces and broilers. Fluidized catalytic cracking regenerators, CO broilers, Coke calciners. Sulphur recovery unit (SRU). Flare systems and Incinerators.
Particulates	Process furnaces and broilers, particularly when firing liquid refinery fuels. Fluidized catalytic cracking regenerators, CO broilers, Coke plants and Incinerators.

In this research, only NO_X reduction will be studied. It will be part of the final refinery optimized planning model to reduce the NO_X emissions. We can summarize our objective of this research into the following points:

- Build a planning model for oil refinery with visbreaker and CDU units based on arab heavy crude oil.
- Quantify NO_X emission from oil refinery for a typical oil refinery consisting of eight processing units.
- Study different options of technologies for NO_X reduction and their effect on cost and profits.
- Application of the developed planning model of the arab heavy crude oil to different cases of NO_X reduction target ranging from 0% to 80%.

- Study the effect of NO_X reduction targets on profits and cost of the oil refinery based on 100,000 BBL of crude oil processed on a daily basis.

Chapter 2

Literature Review

2.1 Overview of Refinery Process

An oil refinery or petroleum refinery is an industrial process plant where crude oil is processed and refined into more useful petroleum products, such as diesel, gasoline, fuel, asphalt base, kerosene, heating oil and liquefied petroleum gas. A crude oil is a mixture containing thousands of different organic hydrocarbon molecules which has about 83-87% carbon, 11-15% hydrogen, 1-6% sulfur and other organic hydrocarbon compounds. Oil refineries are large sprawling industrial plants with extensive piping running throughout, carrying streams of fluids between large chemical processing units. In many ways, oil refineries use much of the petroleum technology and can be thought of as types of chemical plants. The crude oil feedstock has typically been processed by an oil production plant. Usually, there is an oil tank farm at or near an oil refinery for storage of bulk products.

Oil can be used in various of ways because it contains hydrocarbons of varying molecular masses, forms and lengths such as aromatics, paraffins, naphthenes (or cycloalkanes), dienes, alkenes, and alkynes. While the molecules in crude oil include different atoms such as sulfur and nitrogen, the hydrocarbons are the most common form of molecules. Hydrocarbon molecules are molecules of varying lengths and complexity made of hydrogen and carbon atoms, and a small number of oxygen atoms. The differences in the structure of these molecules account for their varying physical and chemical properties, and it is this variety that makes crude oil useful in a broad range of applications.

Once crude oil is separated and purified of any contaminants and impurities, the fuel or the lubricant can be sold without further processing. Octane number of gasoline can be improved by catalytic reforming, which involves removing hydrogen from hydrocarbons producing compounds with higher octane ratings such as aromatics. Intermediate products such as the gas oils can be reprocessed to break heavy, long-chained oil into lighter short-chained ones, by various forms of cracking such as fluid catalytic cracking, thermal cracking and hydrocracking. The final step in the gasoline production is blending of fuels with different octane ratings, vapor pressures, and other properties to meet product specifications.

Oil refineries are large scale plants that are processing about a hundred thousand to several hundred thousand barrels of crude oil on a daily basis. Because of high capacity, many of the units operate continuously, as opposed to processing in batches, at steady state or nearly steady state for months to years. The high capacity makes also process optimization and advanced process control very desirable.

Petroleum products are usually grouped into three categories as follows: light distillates (LPG, gasoline, and naphtha), middle distillates (kerosene, diesel), heavy distillates and residuum (heavy fuel oil, lubricating oils, wax, and asphalt). This classification is based on the way crude oil is distilled and separated into fractions (called distillates and residuum) Below is a list of the main product streams going out from CDU in oil refinery.

- Liquefied petroleum gas (LPG),
- Gasoline (also known as petrol),
- Naphtha,
- Kerosene and related jet aircraft fuels,
- Diesel fuel,
- Fuel oils,
- Lubricating oils,
- Paraffin wax,
- Asphalt and tar,
- Petroleum coke.

The first oil refineries in the world were built by Ignacy Łukasiewicz near Jasło, Austrian Empire (commonly known as Poland) from 1854 to 56, but they were initially small as there was no real demand for refined fuel. As Łukasiewicz's kerosene lamp gained popularity, the refining industry grew.

The world's first large refinery opened at Ploiești, Romania, in 1856-57, with United States investment. After being taken over by Nazi Germany, the Ploiești refineries were bombed in Operation Tidal Wave by the Allies during the Oil Campaign of World War II. Another early large refinery was Oljeön, Sweden (1875). It is now preserved as a museum at a UNESCO World Heritage Site Engelsberg Ironworks.

At sometime, the refinery in Ras Tanura, Saudi Arabia owned by Saudi Aramco was claimed to be the largest oil refinery in the world. For most of the 20th century, the largest refinery was the Abadan Refinery in Iran. This refinery suffered extensive damage during the Iran-Iraq war in the eighties. Currently, the world's largest refinery complex is the Jamnagar Refinery Complex, consisting of two refineries side by side operated by Reliance Industries Limited in Jamnagar, India with a total production capacity of 1,240,000 barrels per day. Now it is time to give a clear description about the main units in a refinery starting with CDU.

2.1.1 Crude Distillation Unit (CDU): The main objective of the CDU unit is to distill and separate valuable distillates (naphtha, kerosene, and diesel) and atmospheric gas oil (AGO) from the crude feedstock. The CDU is using very complex distillation technique. The process starts with preheating of the crude feed utilizing recovered heat from the product streams. Then desalting and dehydrating the crude using electrostatic enhanced liquid/liquid separation (Desalter).

After desalting, the crude oil is pumped through series of heat exchangers and its temperature is raised to about 550 ^{o}F (288 ^{o}C) by heat exchange with product and reflux stream. It is further heated to about 750^{o}F (399 ^{o}C) in a furnace (by direct fired heater, etc…) and charged to the flash zone of the atmospheric fractionators. The furnace discharging temperature is high enough [650 ^{o}F to 750 ^{o}F (343 ^{o}C to 399 ^{o}C)] to cause vaporization of all products withdrawn above the flash zone plus about 10-20 % of the bottoms product. This 10 to 20 % over flash allows some fractionation to occur on the trays above the flash zone by providing internal reflux in excess of the side stream withdrawal. Reflux is provided by condensing the tower overhead vapors and returning a portion of the liquid to the top of the tower, and by pump around and pump back streams in the lower part of the tower. Each of the side stream products removed from the tower decreases the amount of reflux below the point of withdrawal.

Maximum reflux and fractionation is obtained by removing all heat at the top of the tower, but these results in an inverted cone type liquid loading which requires very large diameter at the top of the tower. In order to reduce the top diameter of the tower and even the liquid loading over the length of the tower, intermediate heat removal streams are used to generate reflux below the side stream removal points. To accomplish this, liquid is removed from the tower, cooled by a heat exchanger, and then returned to the tower. Alternatively, a portion of the cooled side stream may be returned to the tower. This cold stream condenses more of the vapors coming up the tower and so increases the reflux below that point.

The energy efficiency of distillation operation is also improved by using pump-around reflux. When enough reflux was produced in the overhead condenser to provide for all side stream draw offs as well as the required reflux, all of the heat energy would be exchanged at the bubble point temperature of the overhead stream. By using pump around reflux at lower points in the column, the heat transfer temperatures are higher and a higher fraction of the heat energy can be recovered by preheating the feed. Although crude towers do not normally use reboilers, several trays are generally incorporated below the flash zone and steams are introduced below the bottom tray to strip any remaining gas oil from the liquid in the flash zone and to produce a high flash point bottoms .The steam reduces the partial pressure of the hydrocarbons and thus lowers the required vaporization temperature. The atmospheric fractionator normally contains 30 to 50 fractionation trays. Separation of the complex mixtures in crude oils is relatively easy and generally 5 to 8 trays are needed for each side stream product in addition to the same number above and below the feed plate. Thus, a crude oil atmospheric fractionation tower with four liquid side stream draw offs is requiring between 30 to 42 trays.

The liquid side stream withdrawn from the tower will contain low boiling components stripped from each side stream in the separate small stripping tower containing 4 to 10 trays with steam introduced under the bottom one. The steam and stripped lighter ends are vented back to the vapor zone of the atmospheric fractionator above the corresponding side draw tray. Overhead condenser on the atmospheric tower condenses the pentane and heavier fraction of the vapors those pass out of the top of the tower. That is the light gasoline portion of the overhead, containing some propane and butanes and all of the higher boiling components in the tower overhead vapor.

Some of this condensate is returned to the top of the tower as reflux, and the remainder is sent to the stabilization section of the refinery gas plant where the butanes and propane are separated from the C5 – 180 ^{o}F (C5 +), LSR gasoline.

Listed below are the the main products from a typical crude distillation unit per their boiling point from lighter to heavier one:

- Fuel Gas: the fuel gas consists mainly of methane and ethane. In some refineries, propane in excess of LPG (Liquefied Petroleum Gas) requirement is also included in the fuel gas stream. This stream is also referred to as dry gas.

- Wet Gas: the wet gas stream contains propane and butanes as well as methane and ethane. The propane and butanes are separated to be used for LPG and, in the case of butanes, for gasoline blending and alkylation unit feed.
- LSR Naphtha: The stabilized LSR naphtha (or light straight naphtha gasoline) stream is desulfurized and used in gasoline blending or processed in an isomerization unit to improve octane before blending into gasoline.
- HSR Naphtha or (heavy straight naphtha gasoline): The naphtha cuts are generally used as catalytic reformer feed to produce high octane reformate for gasoline blending and aromatics.
- Gas Oils: The light atmospheric and vacuum gas oils are processed in a hydrocracker or catalytic cracker to produce gasoline, jet and diesel fuels. The heavier vacuum gas oils can be used as feed stocks for lubricating oil processing units.
- Residuum: The vacuum still bottoms can be processed in a visbreaker, Coker, or deasphalting unit to produce heavy fuel oil or cracking or lube base stocks for asphalt. The residuum can be processed further to produce road or roofing asphalts.

2.1.2 Vacuum Distillation Unit (VDU): The objective of the VDU is to recover valuable gas oils from reduced crude via vacuum distillation. The primary process technique is first to reduce the hydrocarbon partial pressure through vacuum and stripping steam. Then, heat the reduced crude to the desired temperature using fired heaters. Later, flashing the reduced crude in the vacuum distillation column is implemented. After flashing, utilize pump around cooling loops to create internal liquid reflux. Then, products are removed from top, bottom and sides.

2.1.3 Visbreaking Unit: Visbreaking is a relatively mild thermal cracking operation mainly used to reduce the viscosities and pour points of vacuum tower bottoms to meet fuel oil specifications or to reduce the amount of cutting stock required to dilute the cutter stock requirements from 20% to 30% by visbreaking. The gas oil fraction produced by visbreaking is also used to increase catalytic cracker feed stocks and increase gasoline yields.

Long paraffinic side chains attached to aromatic rings are the primary cause of high pour points and viscosities for paraffinic base residual. Visbreaking is carried out at conditions to optimize the breaking of these long side chains and their subsequent cracking to shorter molecules with lower viscosities and pour points. The amount of cracking is limited, since the operation is too severe. The resulting product becomes unstable and forms polymerization products during storage which causes filter plugging and sludge formation. The objective is to reduce the viscosity as much as possible without significantly affecting the fuel stability. For most feedstocks, this reduces the severity to the production of less than 10 % gasoline and lighter materials. The degree of viscosity and pour point reduction is a function of the composition of the residual feed to the visbreaker. Waxy feed stocks achieve pour point reductions from 15 ^{o}F to 35 ^{o}F (-3 ^{o}C to 2 ^{o}C) and final viscosities from 25% to 75% of the feed high asphaltene content in the feed reduces the conversion ratio at which a stable fuel can be made, which results in smaller changes in the properties. The properties of the cutter stocks used to blend with the visbreaker tars also have an effect on the severity of the visbreaker operation. Aromatic cutter stocks such as catalytic gas oils have a favorable effect on fuel stability and permit higher visbreaker conversion levels before reaching fuel stability limitations. The molecular structures of the compounds in petroleum which have boiling points above 1000 ^{o}F (538 ^{o}C) are highly complex and historically have been classified arbitrarily as oils, resins, and asphaltenes according to solubility in the light paraffinic hydrocarbon. The oil fraction is soluble in propane. The resin fraction is soluble in either pentane, hexane, n-heptanes, or octane, depending upon the investigator. Usually either pentane or n-heptane is used. The solvent selected does have an effect on the amounts and properties of the fraction obtained. However, normally little distinction is made in terminology. Many investigators believe the asphaltenes are not in solution in the oil and resins but are very small, perhaps molecular size, solids held in suspension by the resins, and there is a definite critical ratio of resins to asphaltenes below which the asphaltenes will start to precipitate. During the cracking phase some of the resins are cracked to lighter hydrocarbons and others are converted to asphaltenes. Both reactions affect the resin/asphaltene ratio and the resultant stability of the visbreaker tar product serve to limit the severity of the operation. The principal reactions which occur during the visbreaking operation are:

1- Cracking of the side chains attached to cycloparaffin and aromatic rings at or close to the ring so the chains are either removed or shortened to methyl or ethyl groups.
2- Cracking of resins to light hydrocarbons (primarily olefins) and compounds which convert to asphaltenes.

3- At temperatures above 900 ^{o}F (480 ^{o}C), there will be some cracking of naphthene rings. There will be little cracking of naphthenic rings below 900 ^{o}F (480 ^{o}C).

The severity of the visbreaking operation can be expressed in several ways like the yield of material boiling below 330 ^{o}F (166 ^{o}C), the reduction in product viscosity, and the amount of standard cutter stock needed to blend the visbreaker tar to fuel oil specifications as compared with the amount needed for the feedstock. In the United States usually the severity is expressed as the vol% of product gasoline in a specified boiling range, and in the Europe as the wt% yield of gas plus gasoline (product boiling below 330 ^{o}F, or 165 ^{o}C).

There are two types of visbreaker operations, coil and furnace cracking and soaker cracking. The feed is introduced into the system and heated to the desired temperature in the furnace or coil cracking process. The feed is heated to cracking temperature [885 ^{o}F- 930 ^{o}F (474 ^{o}C- 500 ^{o}C)] and quenched as it exits the furnace with gas oil or tower bottoms to stop the cracking.

In the soaker cracking operation, the feed leaves the furnace between 800^{o}F to 820^{o}F (427^{o}C to 438^{o}C) and passes through a soaking drum, which provides the additional reaction time before it is quenched. Pressure is an important design and operation parameter with units being designed for pressures as high as 750 psig (5170 kPa) for liquid phase visbreaking and as low as 100 -300 psig (690kpa -2070kpa) for 20% -40% vaporization at the furnace outlet. For furnace cracking, fuel consumption accounts for about 80% of the operating cost with a net fuel consumption equivalent of

1-1.5 wt% on feed. Fuel requirements for soaker visbreaking are about 30-35 % lower. Many of the properties of the products of visbreaking vary with conversion and the characteristics of the feed stocks. However, some properties, such as diesel index and octane number, are more closely related to feed qualities, and others, such as density and viscosity of the gas oil, are relatively independent of both conversion and feed stock characteristics.

2.1.4 Hydrotreating Process: In hydrotreating, the objective is to remove contaminants (sulfur, nitrogen, metals) and saturated olefins and aromatics to produce a clean product for further processing or finished product sales. The primary process technique is that hydrogenation occurs in a fixed catalyst bed to improve H/C ratios and to remove sulfur, nitrogen, and metals. The first feed is preheated using the reactor effluent. Then hydrogen is combined with the feed and heated to the desired hydrotreating temperature using a fired heater. Later, feed and hydrogen pass downward in a hydrogenation reactor packed with various types of catalyst depending upon reactions desired. The next stage is that the reactor effluent is cooled and enters the high pressure separator which separates the liquid hydrocarbon from the hydrogen/hydrogen sulfide/ammonia gas. Acid gases are absorbed from the hydrogen in the amine absorber. Hydrogen, minus purges, is recycled with make-up hydrogen. Further separation of LPG gases occurs in the low pressure separator prior to sending the hydrocarbon liquids to fractionation.

Some Common Types of Hydrotreating Units are as follows:

Naphtha Hydrotreating: removes sulfur contaminant for downstream processes.

Gasoline Hydrotreating: Sulfur removal from gasoline blending components to meet recent clean fuels specifications.

Mid-Distillate Hydrotreating: Sulfur removal from kerosene for home heating,convert kerosene to jet through mild aromatic saturation and remove sulfur from diesel for clean fuels.

2.1.5 Hydrocracking Process: The objective of the process is to remove feed contaminants like nitrogen, sulfur and metals and to convert low value gas oils to valuable products like naphtha, middle distillates, and ultra-clean lube base stocks. Primary Process technique is the hydrogenation occurs in fixed hydrotreating catalyst beds to improve H/C ratios and to remove sulfur, nitrogen, and metals. This is followed by one or more reactors with fixed hydrocracking catalyst beds to dealkylate aromatic rings, open naphthene rings, and hydrocrack paraffin chains. First of all, preheated feed is mixed with hot hydrogen and passes through a multi-bed reactor with interstage hydrogen quenches for hydrotreating. Later, hydrotreated feed is mixed with additional hot hydrogen and passes through a multi-bed reactor with quenches for first pass hydrocracking. Next is that reactor effluents are combined and pass through high and low pressure separators and are fed to the fractionator where valuable products are drawn from the top, sides, and bottom. Fractionator bottoms may be recycled to a second pass hydrocracker for additional conversion all the way up to full conversion.

2.1.6 Catalytic Reforming Process: The objective of the reforming process is to convert low-octane naphtha into a high-octane reformate for gasoline blending and/or to provide aromatics (benzene, toluene, and xylene) for petrochemical plants. Reforming also produces high purity hydrogen for hydrotreating processes.

The primary process technique is reforming reactions occur in chloride promoted fixed catalyst beds; or continuous catalyst regeneration (CCR) beds where the catalyst is transferred from one stage to another, through a catalyst regenerator and back again. Desired reactions include: dehydrogenation of naphthenes to form aromatics; isomerization of naphthenes; dehydrocyclization of paraffins to form aromatics; and isomerization of paraffins. Hydrocracking of paraffins is undesirable due to increased light ends make. First the process starts where naphtha feed and recycle hydrogen are mixed, heated and sent through successive reactor beds. Each pass requires heat input to drive the reactions. Then, final pass effluent is separated with the hydrogen being recycled or purged for hydrotreating. Reformate product can be further processed to separate aromatic components or be used for gasoline blending.

2.2 Planning and Optimization of Oil Refinery

The main aim of production planning is to decide what to produce, how much to produce and when to produce for a given plan horizon in a company. The production plan includes yearly plan, seasonal plan and monthly plan in terms of time frame. The objective of production planning in oil refinery is to generate many valuable products as possible, such as gasoline, jet fuel, diesel, and so on. Also, at the same time you need to satisfy market demand and other constraints. Oil refining is one of the most complex chemical industries, which involves many different and complicated processes with various possible connections. It is typical for oil refineries to include tens of units. For this reason, the optimization of the production planning of the overall refinery is considered as one of the most difficult and challenging tasks, which is also often formidable, even impossible**.** Nevertheless, the production plan optimization is an important profit growth point. As a result, it also becomes a burning hot topic in both industry and academia. Various optimization models have been developed for individual units with specific technological characteristics. However, the optimization of the production units does not achieve the global economic optimization of the plant. Usually the objectives of the individual units are conflicting and many times infeasible thus many production paths are restricted or disabled. The production planning optimization for refinery-wide has been addressed by using linear programming in the past decades. Although the linear programming models are not good enough to consider the discrete features of the planning problem, such as the dynamic feature of demand, uneven features of the supplement of crude oil and the production of processing units in terms of time periods. Recently, studies for optimization of production planning have been toward the development of nonlinear programming and mixed integer linear programming models**.** There were many studies to propose a production planning model and algorithm for refinery wide optimization as stated in many journals like chemical engineering and research design journal.

Changing in crude petroleum prices, fluctuation in production practices by the petroleum producing countries and changing market demands for different products are main reasons for refiners to resorting advanced decision making strategies. Refinery production planning and scheduling are two such cases affected by market instability. As part of trying to resolve problems coming out from market instability, optimization with LP was included in early studies in oil industry to help in solving such issues.

Linear programming is an approach to the solution of a particular class of optimization problems. It is concerned with finding values for a set of variables which maximize or minimize a linear objective function of the variables, subject to a set of linear inequality constraints. Linear programming was first proposed by Dantzig in (1947), which was mentioned by Edgar (2001), refering the optimization problems in which both the objective function and the constraints are linear. LP problems exhibit the special characteristic that the optimal solution of the problem must lay on some constraints or at the intersection of several constraints. Dantzig was the first to propose the most popular algorithm in LP called the simplex algorithm.

Despite the many contributions those have been reported on planning models, very few can be found that specifically address the petroleum refining industry. Symonds (1956) developed an LP model for solving a simplified gasoline refining and blending problem. The advantage of LP is its quick convergence and useful of implementation. Allen (1971) presented in his paper an LP model for a simple refinery that consists mainly of three units: distillation, cracking and blending.

Optimization, particularly linear programming (LP), has been traditionally used for such purposes. Other optimization algorithm such as non linear programming (NLP) and mixed integer have been introduced. Since the introduction of LP in the 1950, the optimization of production planning has become possible with non linear algorithms but still the preferred method is LP. Symonds and Manne applied LP to long term supply and production planning of crude oil processing. Moreover availability of commercial software has increased use of this approach to real life problems. Due to complexity of NLP algorithms, their use in plant wide problems is limited and consequently previous studies have dealt with application of mixed integer Liner programming (MILP) algorithms to such problems. Zhang et al (2007) considers a refinery as a combination of process system and utility systems and develop a MILP algorithm for better energy utilization. Lundgren et al used a MILP algorithms to optimization of scheduling and production planning of one distillation unit and two hydro treatment units. Ready et al used a MILP for short term optimization of scheduling of refinery operations such as receiving crude from large crude carriers to the storage and CDU units. The plant is divided into subsystems. When these subsystems are coupled, it allows development of the representation of the main scheduling activities to develop new strategies. The new strategies will be incorporated in an automated planning and scheduling system. Hence, the planning system will bring out scheduling system that generates short term schedules.

Since planning and scheduling activities in oil refineries is introduced, the potential benefits of optimizations for process operations in oil refineries with applications of linear programming in crude blend and product pooling have long been observed Symonds (1955).

Planning in refinery has old histories which is worth mentioning in order to understand the work done before in the area of oil refinery planning. A number of contributions can be found in many of the science and engineering journals that consider design and planning over a long-term horizon. Sahinidis et al. (1989) presented a multiperiod mixed integer linear programming (MILP) model whose decisions are to incorporate process design and capacity expansion and proposed four strategies to handle model complexity. Sahinidis and Grossmann (1991) improved the performance of the same model through reformulation. Varvarezos et al. (1992) developed an outer-approximation method to solve convex nonlinear programming (NLP) and mixed integer nonlinear programming (MINLP) for multiperiod design problems. Boding ton (1992) also mentioned the lack of systematic methodologies for handling nonlinear blending relations.

Production planning is a discipline related to the macro-level problem of allocation of production total capacity and production time with less emphasis on the raw materials, intermediate products, and final product inventories; as well as labor and energy resources. Its primary objective is to determine a feasible operating plan consisting of production goals that will optimize a suitable economic criterion. Typically, over the course of a few months to a few years.

Cox head (1994) identifies several applications of planning models in the refinery and oil industry, such as crude selection, crude allocation for raw material supply and planning. Given marketing forecasts for prices, market demands for products, and considerations of equipment availability and inventories. In essence, planning fundamental function is the development of a good set of operating goals for the future period. In the present settings of the oil and gas or hydrocarbon industry, planning requirements have become increasingly more difficult. The demend is arising of the need to produce more varied, higher-quality products while simultaneously meeting increasingly tighter environmental legislations and policies as it has been reported by Fisher and Zellhart Bodington (1995).

On the other hand, production scheduling, in the context of the chemical processing industry, deals with micro-level problems embedded in production planning problems. Production scheduling involves deciding on the methodology that determines the feasible order or sequence and timing in which various products are to be produced in each piece of equipment. Final product should meet the production goals that are laid out by the planning model. Major objective of chemical processing industry is to efficiently utilize the available equipment among the multiple types of products to be manufactured, to an extent necessary to satisfy the production goals. This can be achieved through optimizing a suitable economic or systems performance criterion, typically, over a short term horizon ranging from several shifts to several weeks. Scheduling functions specify the task(s) of each stage of production and this includes defining and projecting the inputs and outputs from each production operation. It is particularly required whenever a processing system is used to produce multiple products by allocating the available production time between products as reported by Sahinidis et al (1989), Birewar et al (1995) and Bodington (1995).

Fisher and Zellhart, Bodington (1995), also emphasize that a planning model differs from a daily schedule model or an operational process controller. For example, they pointed out that the product or process yields predicted or estimated in the planning model should not be expected to be used exactly in executing operating conditions. This is because planning models are almost always an average over time and not an accurate prediction of process conditions at any particular instant. As opposed to planning models, operations are not averaged over the scheduling period as time and operations move continuously from the beginning of the particular period to the end. The schedule is revised as needed by operation team so that it always starts from what is actually happening with revisions typically occur on each day or on each shift.

There are few commercial tools for production scheduling and these do not allow a rigorous representation of plant particularities, Rigby Et al (1995). For this reason refineries are developing in house tools strongly, to obtain essential information for a given system. In many of the operational research journals, there are specific applications based on mathematical programming such as crude oil unloading and gasoline Blending Bodington (1992).

Liu and Sahinidis (1996) proposed a cutting plane algorithm that exhibits fast convergence. Liu and Sahinidis (1997) presented a planning model where forecast parameters are assumed to be unclear. Still working on the long-range horizon of planning process networks, Iyer and Grossmann (1998) proposed a bi-level decomposition whereby the first step solves a design problem followed by the solution of an operation and expansion problem subject to the previous results. The same methodology was applied to solve a MILP formulation developed for synthesis and operation planning of utility systems over a long-term horizon, Iyer and Grossmann (1998). Bok et al (1998) formulated a long-range capacity expansion planning model for chemical processing networks that considers uncertain demand forecast scenarios.

Increasingly, oil refinery management is concerned with improving the planning of their operations. The major factor, among others, is the dynamic nature of the economic environment. Companies must assess final product specifications, prices and crude oil compositions or even be able to explore immediate market opportunities, Magathaes et al (1998).

The chemical processing industry had to restructure in order to compete successfully in this new scenario where better economic performance with more efficient plant operation has been achieved, Moro et al (1998). Implementation of advanced control system in oil refineries generated significant gains in productivity of the plant units. These results increased the demand for a more complex automation system that takes into account production objectives; as a result, unit optimizers were introduced. Nevertheless, the optimization of production units does not assure the global economic optimization of the plant. The objective of individual units are usually conflicting and thus contributes to sub optimal and many times infeasible operation. The lack of computational technology for production scheduling is the main obstacle to the integration of production objective into process operations, Barton et al (1998). A more efficient approach would incorporate current and future constraints in the synthesis of production schedules. The short term production objective must be translated into operating condition for the processing units. Such an approach supplies an analytical tool for the effect of economic disturbances in the performance of the production system and provides mechanisms to account for commercial and technological uncertainties.

Ramage (1998) refers to nonlinear programming (NLP and MINLP) as a necessary tool the refineries of the 21 century, as a result of the significant progress made in the nineties. Hartmann (1998) stresses on the differences between a planning model and scheduling model. In general, process manufacturing planning models consider economics of the operations by handling issues of what to do and how to do it. In the other hand, whereas process manufacturing scheduling models consider feasibility of the operations by addressing the issues of when to do it. In particular, planning models ignore changeovers and treat products in groups of families. Conversely, scheduling models explicitly consider changeovers and consider products in greater detail, including the shipment of specific orders for specific products to specific customers.

Alireza (2006) extended the LP approach to the optimal Simplex tableau, where he proposed an original two-stage methodology based on the marginal contribution of oil products and the production elasticity of unit processes to provide an additive CO_2 allocation scheme. We show that this procedure emerges from the equilibrium behavior of the refinery and is consistent with microeconomic theory.

As it was mentioned in the previous chapter, oil refinery has hundreds of chemical units which are working simultaneously in a very complicated way. The aim of refinery operation is to generate as much profit as possible by converting crude oils into more profitable products. Mathematical optimization has become indispensable tools to realize this goal. Linear programming (LP) is the most widely used technique in refinery operation optimization, which is called planning and scheduling in industry. The main goal in planning is to determine high-level decisions such as production levels and product inventories for given marketing demands.

One of the first contributors to consider nonlinearity in production planning is that of Moro et al. (1998). The main objective of their study was to develop a nonlinear planning model for refinery production. The model represented a general refinery topology and a real world application was developed for the planning of diesel production in one of the refineries in Brazil. The model was solved and the results were compared to the current situation where no computer algorithm was being used. Pinto and Moro (2000) developed also a nonlinear planning model for refinery production. The model represents a general petroleum refinery and its framework allows for the implementation of nonlinear process models as well as blending relations. This model assumes the existence of several processing units, producing a variety of intermediate streams, with different properties, that can be blended to constitute the desired kinds of products. However, the model was based on assumption that many of the refinery processes are linear which affect the overall predictability of the model.

Van den Heever and Grossmann (1999) used a disjunctive multiperiod approach, which incorporates design, operation, and expansion planning. The availability of LP based commercial software for refinery production planning, such as PIMS (Process Industry Modeling System), has allowed the development of general production plans for the whole refinery which can be interpreted as general trends. The major advance in this area is based on model refinement, notably through the use of nonlinear programming, as in picaseno- gamiz (1989) and more recently, Moro et al (1998. 2000).

During 2000, Pinto et al. (2000) made a discussion on planning and scheduling application for oil refinery operations which is an improvement of Moro model. They presented a nonlinear planning model in the first part similar to the one developed by Moro et al. (1998). In the second part, they addressed scheduling problems in oil refineries that are formulated as mixed integer optimization models and relied on both continuous and discrete time representations. They have considered the development and solution of optimization models for short term scheduling of a set of operations including products received from processing units, storage and inventory management in intermediate tanks, blending in order to attain oil specifications and demands, and sequence transporting in oil pipelines. They have also reported important real-world examples on refinery production and distribution. The diesel distribution problem at one refinery in Brazil and the production problems related to fuel oil, asphalt and LPG was addressed. Zhang and Zhu (2000) showed in their paper a novel decomposition strategy to tackle large scale overall refinery optimization problems. The approach is derived from an analysis of the mathematical structure of a general overall plant model. This understanding forms the basis for decomposing the model into two levels. These levels are the site level (Master Model) and the process model (submodels). The master model determines common issues among the processes. Then, submodels optimize individual processes. The results from these submodels are fed back to the master model for further optimization. Zhang et al. (2001) studied a simultaneous optimization strategy for overall integration in refinery planning. They have presented a method for overall refinery optimization through integration of the hydrogen network and the utility system with the material processing system. In order to make the problem of overall optimization solvable, the current practice adopts the decomposition approach, in which material processing is optimized first using linear programming (LP) techniques to maximize the overall profit. Then, supporting systems, including the hydrogen network and the utility system, are optimized to reduce operating costs for the fixed process conditions determined from the LP optimization.

Sahinidis (2003) discussed the importance and challenges associated with modeling uncertainty in process operations and provided an overview of theory and methodology involving uncertainty. Neiro and pinto (2004) presented a general MINLP model for petroleum supply chain with storage tanks and pipelines interconnected by intermediate streams, starting with processing units which were based on the model developed by Pinto et al. (2000).

Lately, Li et al. (2005) conducted a thorough study on integrating crude distillation, FCC and product blending modules into refinery planning models. They have presented a refinery planning model utilizing simplified empirical nonlinear process models with considerations for crude characteristics, products yields and qualities.

Also, Neiro and pinto (2005) studied multi-period optimization for production planning of petroleum refineries. The given model given is based on a nonlinear programming formulation that was developed to plan the production over a single period of time. Uncertainties related to petroleum and product prices as well as demand is then included as a set of discrete probabilities. Further work in optimization continued with considering refineries emission like SO_2 and CO_2.

Ba shammakh (2007) has developed a mathematical model for oil refinery planning with CO_2 reduction using MINLP. He also has developed a mathematical model for oil refinery planning and optimization with SO_2 reduction using MINLP.

2.3 Overview of Technology for NO_X Emission Control

Nitrogen dioxide (NO_2) is a group of highly reactive gasses known as "oxides of nitrogen," or "nitrogen oxides (NO_X)." Other nitrogen oxides include nitrous acid and nitric acid. While EPA's National Ambient Air Quality Standard covers this entire group of NO_X, NO_2 is the component of greatest interest and the indicator for the larger group of nitrogen oxides. NO_2 forms quickly from emissions from cars, trucks and buses, power plants, and off-road equipment. In addition to contributing to the formation of ground-level ozone, and fine particle pollution, NO_2 is linked with a number of adverse effects on the respiratory system.

EPA (Enviromental protection Agency) first set standards for NO_2 in 1971, setting both a primary standard (to protect health) and a secondary standard (to protect the public welfare) at 0.053 parts per million (53 ppb), averaged annually. The agency has reviewed the standards twice since that time, but chose not to revise the standards at the conclusion of each review. All areas in the U.S. meet the current (1971) NO_2 standards.

The Clean Air Act requires EPA to set national ambient air quality standards for "criteria pollutants." Currently, nitrogen oxides and five other major pollutants are listed as criteria pollutants. The others are ozone, lead, carbon monoxide, sulfur oxides, and particulate matter. The law also requires EPA to periodically review the standards and revise them if appropriate to ensure that they provide the requisite amount of health and environmental protection and to update those standards as necessary. Current scientific evidence links short-term NO_2 exposures, ranging from 30 minutes to 24 hours, with adverse respiratory effects including airway inflammation in healthy people and increased respiratory symptoms in people with asthma.

Also, studies show a connection between breathing at elevated short-term NO_2 concentrations, and increased visits to emergency departments and hospital admissions for respiratory issues, especially asthma. NO_2 exposure concentrations near roadways are of particular concern for susceptible individuals, including people with asthmatic. The sum of nitric oxide (NO) and NO_2 is commonly called nitrogen oxides or NO_X. Other oxides of nitrogen including nitrous acid and nitric acid are part of the nitrogen oxide family. NO_X react with ammonia, moisture, and other compounds to form small particles. These small particles penetrate deeply into sensitive parts of the lungs and can cause or worsen respiratory disease, such as emphysema and bronchitis.

Ozone is formed when NO_x and volatile organic compounds react in the presence of heat and sunlight. People with lung diseases such as asthma, and people who work or exercise outside are at risk for adverse effects from ozone. Risks include reduction in lung function and increased respiratory symptoms such as as respiratory-related emergency department visits, hospital admissions, and possibly premature deaths.

Usually, emissions that lead to the formation of NO_2 also lead to the formation of other NO_X. Emissions control measures leading to reductions in NO_2 is expected to reduce population exposures to all gaseous NO_x. This may have the important co-benefit of reducing the formation of ozone and fine particles both of which pose significant public health threats. Many technologies have been invented for NO_X reduction. Selective Catalytic Reduction is one of the leading technologies in the USA for oil refinery NO_X reduction. SCR will be discussed in details in the next section.

2.3.1 Selective Catalytic Reduction (SCR)

Selective catalytic reduction is a mean of converting nitrogen oxides, also referred to as NO_X with the aid of a catalyst into diatomic nitrogen, N_2, and water. A gaseous reluctant, typically anhydrous ammonia, aqueous ammonia or urea, is added to a stream of flue or exhaust gas and is absorbed onto a catalyst. Carbon dioxide, CO_2 is a reaction product when urea is used as the reductant.

Selective catalytic reduction of NO_X using ammonia as the reducing agent was patented in the United States by the Engelhard Corporation in 1957. Development of SCR technology continued in Japan and the US in the early 1960s with research focusing on less expensive and more durable catalyst agents. The first large scale SCR was installed by the IHI Corporation in 1978.

Commercial selective catalytic reduction systems are typically found on large utility boilers, industrial boilers, and municipal solid waste boilers and have been shown to reduce NO_X by 70-95%. More recent applications include diesel engines, such as those found on large ships, diesel locomotives, gas turbines, and even automobiles.

Advantages and disadvantages of SCR:

SCR has higher NO_X reductions than low-NO_X burners and selective Non-Catalyctic Reduction (SNCR). It is also applicable to sources with low NO_X concentrations. Reactions occur within a lower and broader temperature range than SNCR. The SCR unit does not require modifications to the combustion unit.

On the other hand, SCR significantly has higher capital and operating costs than low-NO_X burners and SNCR. Retrofit of SCR on industrial boilers is difficult and costly. The SCR requires a large volume of reagent and catalyst. SCR may require downstream equipment cleaning. In addition, it also results in ammonia in the waste gas stream which may impact plume visibility, and resale or disposal of ash.

Beginning with diesel engines manufactured on or after January 1, 2010, the engines at the US are required to meet lowered NO_x standards. All of the heavy duty engine (Class 7-8 trucks) manufactures, except for Navistar International, continuing to manufacture engines after this date have chosen to utilize SCR. This includes Detroit Diesel (DD13, DD15, and DD16 models), Cummins (ISX line), PACCAR, and Volvo/Mack. These engines require the periodical addition of Diesel Exhaust Fluid (DEF- a urea solution) to enable the process. DEF is available in a bottle from most truck stops, and sometimes have put in bulk DEF dispensers near the Diesel Fuel pumps. Navistar has chosen to utilize Enhanced Exhaust Gas Recirculation (EEGR) to comply with the Environmental Protection Agency (EPA) standards.

2.3.2 Selective Non – Catalytic Reduction (SNCR)

SNCR is a process to blow NH_3 into the boiler section where the exhaust gas temperature is 850 ^oC-950 ^oC and breakdown NO_X into N_2 and H_2O without the use of a catalyst. Despite the advantages of not requiring a catalyst and its lower installation costs, NO_X removal efficiency is as low as 40% at an NH_3/NO_x molar ratio of 1.5. Because of this, it is used in regions or equipment where there is no need for a high NO_x removal efficiency. More NH_3 is also leaked than with the selective contact reduction method, requiring measures to cope with NH_4HSO_4 precipitation in the event of high SO_3 concentrations in the exhaust gas. This technology is mainly used at small commercial boilers and refuses incinerators. With respect to thermal power plant applications, this technology has only been installed at Chubu Electric Power's Chita thermal power plant No. 2 unit (375kw) in 1997.

For about 20 years SNCR systems have been used in waste incineration plants, and rather occupied a niche position in the nineties. This was mainly due to lacking experience with this fairly new process, which made approval processes rather difficult and delayed them in an incalculable manner. Usually, operators were more interested in getting a speedy approval than in cost effectiveness, and therefore they mostly chose systems where least resistance was expected in the approval process. Rethinking started with the slow-down of the economy at the end of the nineties. Biomass plants, which are also operated under the same regulations are subjected to a much higher cost pressure. Because of that, solutions are preferred that fulfill all technical requirements of the regulations and are more cost-effective, instead of searching for the maximum technical solutions for these systems. In biomass incineration plants, the SCR technology practically does not play any major role. Furthermore, most of the waste incineration plants have been equipped with SNCR systems since the year 2000. Discussions about a reduction of the emission limit values for waste incineration plants have also challenged the NO_x limit values. Currently, the draft of the 37th BlmSchV in Germany aims at NO_x limits of <100 mg/Nm³ compared to the currently valid 200 mg/Nm³. In this connection, it is believed that clean gas values of < 100 mg/Nm³ with an acceptable NH_3 slip can only be obtained in a SCR process, It means the end to the SNCR technology for waste incineration plants if this opinion prevails. In a selective non-catalytic reduction (SNCR) process of nitrogen oxides, reductants in an aqueous solution (ammonia water, urea) or in gaseous form (ammonia) are injected into hot flue gases. Following the overall post-combustion reactions for urea,

$$NH_2CONH_2 + 2NO + ½O_2 = 2N_2 + NO_x + 2H_2O$$

or for ammonia molecular nitrogen, water and carbon dioxide are formed as per below equation.

$$4NH_3 + 4NO + O_2 = 4N_2 + 6H_2O$$

The optimum temperature range, where a noticeable NO_x reduction is achieved, is between 900 and 1,100 °C depending on the composition of the flue gas. Above this temperature range ammonia is oxidized to an increasing extent and nitrogen oxides are formed. At lower temperatures the reaction rate is slowed down, causing an ammonia slip which may result in the formation of ammonia salts in the further flue gas path and may lead to secondary problems. Therefore, the ammonia slip should be kept on a minimum. These chemical reactions are similar if catalysts are used and also take place in a limited temperature window which, however, is in a range outside the furnace or the boiler.

2.3.3 Gas Conditioning Technology (GCT)

The reduction of emission through the design and implementation of the appropriate combustion system is essential to offering maximum operational benefits. The ability to offer emission reduction through the use of the latest combustion technology promotes a method that achieves maximum emissions reduction, while avoiding the cost and complexity of back-end cleanup systems. Choosing the right system based on the operating conditions, furnace design, fuel supplies, and other mitigating factors is critical to implementing a successfully operating system. By addressing all the aspects of the combustion process, the entire combustion system can be optimized to produce the lowest possible emissions.

The gas conditioning involves a fuel dilution process whereby boiler flue gases are induced and mixed with the existing refinery gas fuel to generate a low BTU gas. The fuel dilution reduces thermal NO_x by reducing the flame temperature and lowering the local oxygen concentration. Since it also increases the fuel mass flow, it improves fuel-air mixing, reduces the residence time under NO_x forming conditions, and homogenizes the flame, which serves to further lower the peak flame temperature. Fuel delution technology also reduces the carbon radical concentrations in the combustion zone and thereby reduces prompt NO_x formation.

The Chevron refinery in Richmond, California needed to reduce their total plant NO_x emissions to come into compliance with new local air quality regulations. An initial baseline survey of NO_x emissions at the refinery indicated that the five utility boilers in their Power Plant #1 contributed about 25% of the total refinery NO_x emissions, with observed NO_x emissions levels ranging from 250 to 450 ppm. New regulations required then to reduce the NO_x emissions on these boilers to less than 27 ppm. Initial planning called for the use of Selective Catalytic Reduction (SCR) to meet these requirements. Close cooperation between Chevron’s NO_x Reduction Project Team, consultants, and equipment suppliers resulted in an alternate solution using new burners equipped with GCT. After initial testing on one unit it was demonstrated that the required NO_x levels could be sustained without the addition of SCR’s and the remaining units were subsequently converted. Successful application of this technology on all five boilers resulted in over 90% NO_x reduction, allowing all the boilers meet the targeted limit and resulting in substantial cost savings.

2.3.4 NO_x-Reduction by Oil/Water Emulsification

Within the recent years, much work has been done on the influence of water on NO_x emission levels. Various fuel : water volumetric ratios from 1:1 to 19:1 have been tested for combustion properties. In most cases, volume percent surfactant was added for emulsion stabilization.

An emulsion is a mixture of generally immiscible liquids (phases), such as oil and water. During the process of emulsification, the disperse phase (water) is introduced into the liquid phase (oil). By the application of high shear, the particle size (droplet size) of the disperse phase is reduced. The smaller the particle size, the more stable is the generated emulsion. Additional stability can be achieved by the introduction of surfactants or stabilizers.

Approx. 90% of the NO_X resulting from the fuel combustion process is NO (Nitrogen Oxide). The NO is primarily formed by the oxidation of atmospheric nitrogen (N_2). Water added to the fuel lowers the combustion temperature due to water evaporation. When the water in the fuel-water emulsion evaporates, the surrounding fuel is vaporized, too. This increases the surface area of the fuel. Lower temperature and better fuel distribution leads to a lower formation of NO_X.

Introducing water into the fuel combustion has been shown in many functions to lower the NO_X emissions. Water can be added by forming a fuel/water emulsion in the following two ways:

- unstabilized emulsion: Inline emulsification of water into the fuel prior to injection.
- stabilized emulsion**:** Manufacture of a stable fuel/water emulsion to be used as a drop-in fuel alternative.

Ratio for both stabilized and unstabilized emulsions are as follow:

Unstabilized emulsion ratio

water added vol%: 10 to 80%

NO_x reduction by: 4 to 60%

Stabilized emulsion ratio

water added vol%: 25 to 50%

NO_x reduction by: 22 to 83%

Canfield (1999) summarizes the NO_X reduction by the use of water and other additives.

2.3.5 Oxygen-Enhanced Combustion

Praxair, Inc and its partners have developed a novel oxygen-based technology that can reduce NO_X emissions from fired boilers, while improving combustion characteristics such as loss-on ignition (LOI). This novel technology replaces a small fraction of the combustion air with oxygen. In order to support this concept, Praxair is also developing an oxygen transport membrane (OMT) process that uses pressurized ceramic members for separation of oxygen from air.

Testing was conducted using Power's pilot-scale combustion facility. The experiments demonstrated that the concept of oxygen-enhanced low NO_X combustion could meet the emissions target of 0.15 lb/MMBtu with minimal impact on CO emissions and furnace performance. The pilot-scale test facility is a water-cooled tunnel furnace designed to test burners up to 50 MMBtu/hr firing rate with time-temperature histories similar to full-scale PC-fired boilers. The test facility has two locations for separated over-fire air (SOFA) injection. The burner was designed for a firing rate of 26 MMBtu/hr and was typically fired at 24 MMBtu/hr for these.

An eastern bituminous coal, Mingo Logan, was then used in Phase I-B evaluating both the effect of a lower volatile coal and the effect of oxygen addition method. During Phase II, selected experiments were repeated with the Illinois No. 6 experiments showing that even when the baseline (air only) emissions are very low, oxygen addition can drive the NO_X emissions even lower. Furthermore, the overall data further show the reductions are relatively independent of the initial NO_X concentration. Data from the Mingo Logan experiments show that the concept works even with the lower volatile coal, and within that technique the oxygen has a large impact on NO_X reduction.

In addition to the reduction in NO_x, benefits can be achieved in the areas of reduced LOI and opacity, increased boiler efficiency, and reduced fan limits. Subsequent testing at two utility boilers, City Utilities’ James River Unit 3 and Northeast Utilities’ Mt. Tom Generating Station, has demonstrated these benefits of the technology while decreasing NOx emissions. Preliminary economic analysis indicates that cost saving of 50% can be realized when compared to SCR.

CHAPTER 3

Model Development for Oil Refinery

3.1 Mathematical Model Development

In this section, a general mathematical model for an oil refinery is developed. The objective of this model is to maximize profit from selling the final products with specifications subject to reducing NO_X emissions to a certain target using the different mitigation options presented in the chapter one.

Prior to the master model development, which includes all units under consideration as shown in Figure 3.1, a model is developed for each unit (sub-models).

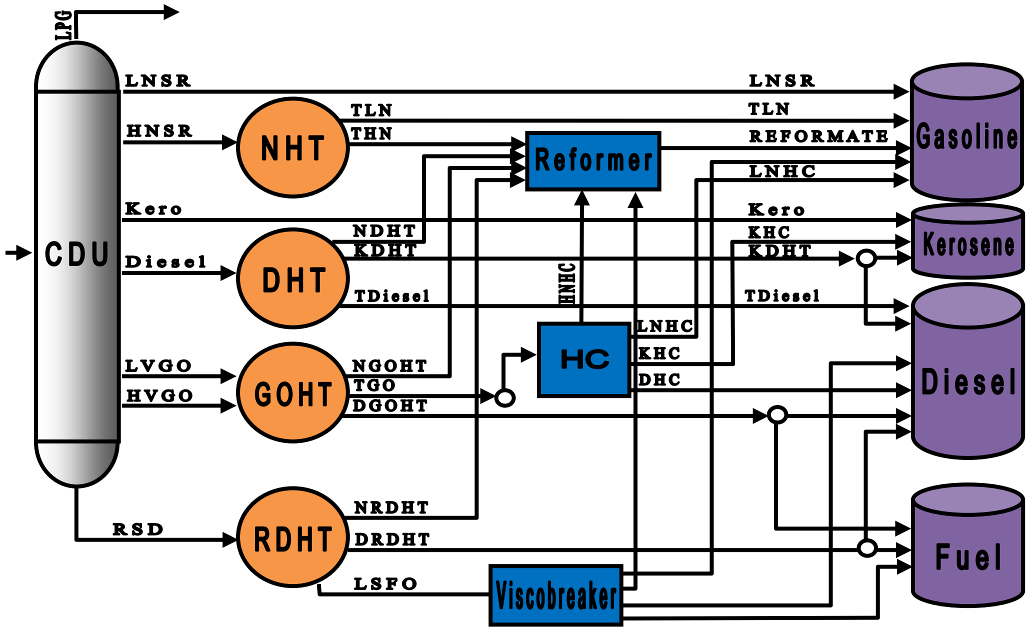


Figure 3.1: Oil refinery layout showing all main process units

In total, there are eight major units and different blending pools. After developing the sub-model for each unit, they are connected together by specifying an outlet of one unit as inlet for the following unit. For simplicity, only the CDU model is shown in details as an example and a general model is given after.

The CDU model can now be summarized as follows:

$$v_p = \sum_{k=0} a_k \, (T_p)^k \qquad \forall \; p \in P_{CDU} - \{Rsd\} \tag{3.1}$$

v_p represents the total volume percent vaporized (volume %) from the crude at cut temperature T_p for product p, except the residual product, of the CDU unit (P_{CDU} is the set of all CDU products). The volume % is a polynomial function in product cut-point T_p which is equivalent to the end point temperatures (EP). The product cut-point T_p or end point temperature (EP) is the temperature at which a given fraction or cut will be vaporized.

Since the last cut is the residual of the crude, it will be assumed that the accumulative vaporized percent will be 100%. The residual cut volume percent will be expressed as:

$$v_{p=Rsd} = 100 \tag{3.2}$$

For each product, cut and volume flow rate is calculated from subtracting its volume percent vaporized from the previous cut and multiply the product with the crude feed to the CDU:

$$V_{CDU,p} = F_{CDU} * \left(\frac{v_p - v_{p-1}}{100} \right) \qquad \forall p \in P_{CDU} - \{Rsd\} \tag{3.3}$$

$V_{CDU,p}$ represents the volume flow rate of all the product streams (p) from the CDU unit. Where the F_{CDU} is the crude oil feed to the CDU unit.

Properties of each product from the CDU (API, sulphur etc.) are polynomial functions of mid-volume percent vaporized of the concerned product. Mid-volume for any product can be calculated from averaging the accumulative current cut volume percent with the previous cut volume percent vaporized as will be shown below.

$$X_{CDU,p} = \sum_{k=0} a_{k,x} \left(\frac{v + v_{p-1}}{2} \right)_p^k \qquad \forall p \in P_{CDU}, x \in X_p \tag{3.4}$$

$X_{CDU,p}$ represent different properties (x) for each product (p) from the CDU unit. X_p is the set of all the properties calculated for the specified product stream (p).

$$V_{CDU,p} = \sum_{m \in M} V_{CDU,p,d} \qquad \forall \; p \in P_{CDU} \tag{3.5}$$

$V_{CDU,p,d}$ represents the volume flow rate of all the streams split from the CDU products (p) to different destinations (d).

All fractions for the CDU, except the residual, have upper and lower limit for their cut-point:

$$T^{L}_{CDU,p} \;\leq\; T_{CDU,p} \;\leq\; T^{U}_{CDU,p} \quad \forall p \in P_{CDU} - \{Rsd\} \tag{3.6}$$

$T_{CDU,p}$ is the cut-point temperature for product (p) of CDU unit.

Also, the crude feed to the unit cannot exceed its throughput capacity:

$$F_{CDU} \;\leq\; Umax_{CDU} \tag{3.7}$$

Other sub-models for hydrotreaters, reformer and HC are developed with the aid of available correlations in the literature for the given units to calculate products amount with properties (Baird, 1987). Theses sub-models are coded in GAMS and are shown in Appendix B.

3.2 Modeling of CDU for Arab Heavy Crude Oil (Saudi Arabia)

The main products from CDU are:

- LPG (liquefied petroleum gas)
- LNSR (light naphtha straight run)
- HNSR (heavy naphtha straight run)
- Kerosene

- Diesel
- LVGO (light vacuum gas oil)
- HVGO (heavy vacuum gas oil)
- Residual

The data in table 3.1 are taken from Research & Development Center from Saudi Aramco Company. The mid volume is calculated based on the following formula:

Mid Volume % = (Current Point Volume% + Previous point Volume %) / 2.0.

The data from R&D center in Saudi Aramco Company is the result of many years of experimental work executed through a small distillation unit in their laboratory. After calculating the mid volume, we should be able to get two more plots. The first one represents the volume percentage of crude oil evaporated or removed versus the cut point temperature (End Point Temperature). Admittedly, we can fit the data using Excel sheet to three or four degree polynomial. The second plot will be to plot API versus mid volume.

Table 3.1: Arab Heavy Crude Oil Data for Volume% Removed Versus Cut temperature

Cut Temperature (F)	Volume of Crude Removed %	Mid. V. %	API
100	1.8	0.9	
200	7.4	4.6	77.6
315	16.7	12.05	61.2
400	23.8	20.25	49.7
500	33	28.4	41.9
600	41.7	37.35	35
700	50.3	46	28.4
800	58.7	54.5	23.8
800	66	62.35	19.9
1050	76.4	71.2	16.3
1200	100	88.2	2.6

As shown in the figure 3.2, the fitted data shows a two degree polynomial. The given polynomial in figure 3.2 was reduced from four to two degree polynomial since the coefficients of other terms are as small as 10^{-5}. So, now we have a model equation that is nonlinear which represent the percentage of crude volume removed at any desired cut temperature. That way, we can calculate how much are the quantity of each cut as long as we know the feed flow rate and the cut temperatures of the desired cut and the previous one using the model equation given in figure 3.2. Equation (3.8) shows the reduced form of the volume% vs cut temperature to the second degree polynomial.

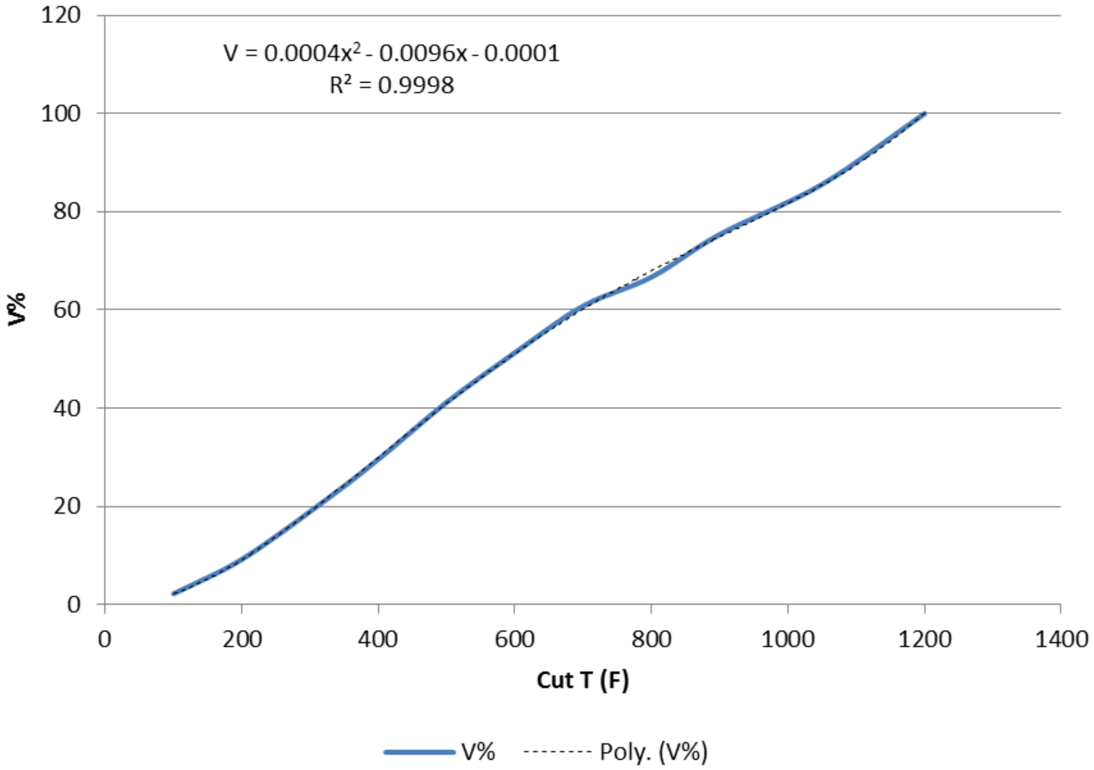


Figure 3.2: Accumulative Volume % removed vs Cut Temperature for AH Crude Oil

$$V = 0.0004x^2 - 0.0096x - 0.0001 \quad R^2 = 0.9998 \tag{3.8}$$

The second plot that we can obtain from the Table 3.1 is the API plot which is a function of the mid volume% of crude oil. Figure 3.3 below shows the data from table 3.1 plotted for API versus the mid volume % calculated using the mid volume formula mentioned earlier. The mid volume is a crude oil property that one ought to model and study. As done earlier and using a three degree polynomial, we obtain, as you can see from figure 3.3, a three degree polynomial where the small coefficients terms, fourth power term and above (less that 10^{-5}), have b been removed. Inadvertently, now we can get the API of the crude oil knowing its mid volume. Equation (3.9) shows the API versus mid volume % relationship in a mathematical reduced form to the second degree polynomial.

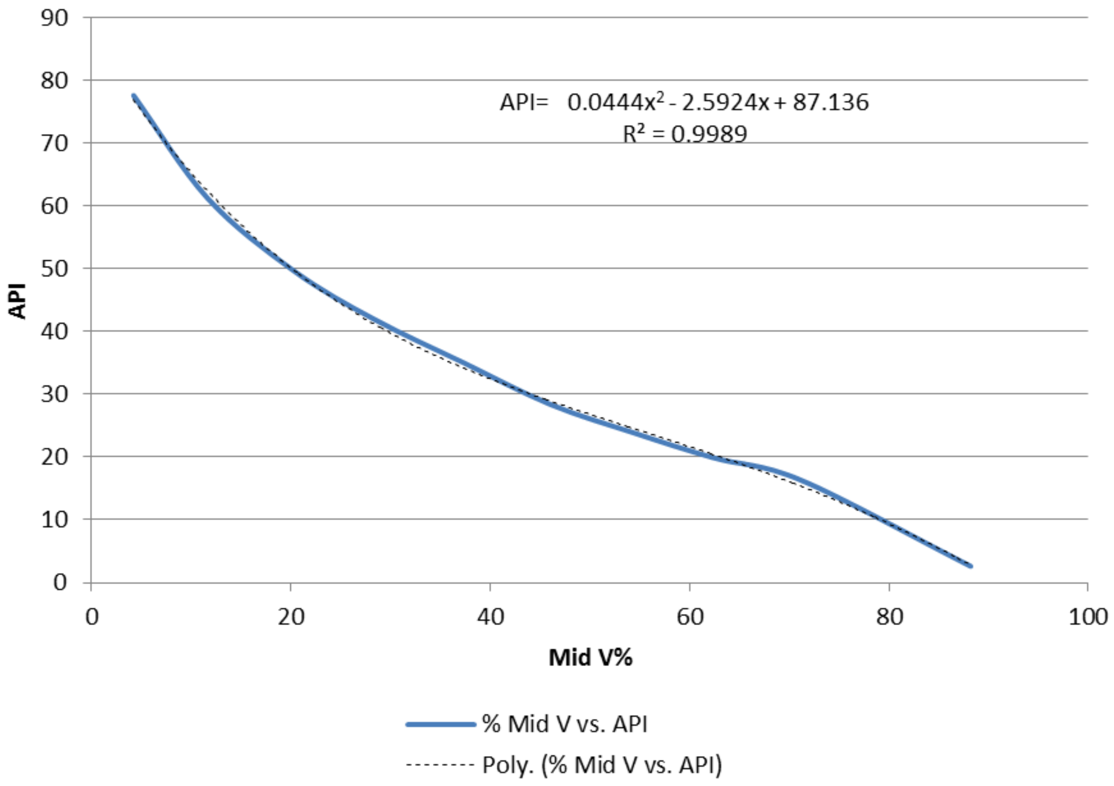


Figure 3.3: API as a function of mid. V% for Arab Heavy Crude Oil

$$\text{API}= \quad 0.0444x^2 - 2.5924x + 87.136 \qquad R^2 = 0.9989 \tag{3.9}$$

Another two important properties to be considered are the nitrogen and sulphur contents in the crude at each cut temperature. The data in table 3.2 have been collected from Ras Tanurah laboratory Division in Saudi Aramco Company.

Table 3.2: Arab Heavy Crude Oil Data for Nitrogen & Sulfur Contents Versus cut Temperature

Cut Temperature (F)	Nitrogen Content ppm	Sulfur Content Wt. %
200	0.5	.0031
340	0.5	0.024
450	0.5	0.175
700	44	1.69
800	670	3.08
900	860	3.49
1050	1043	3.75
1200	4833	4.38

We used the above data to produce two plots. Similar to what we have done earlier with API and volume % removed of crude oil models, here we used the three degree polynomial fit to the data above on an Excel sheet for the nitrogen plot. The output for the nitrogen data, as shown below in figure 3.4, is very close to third degree polynomial since the terms after the third order are very small and can be truncated (less than 10^{-6}).

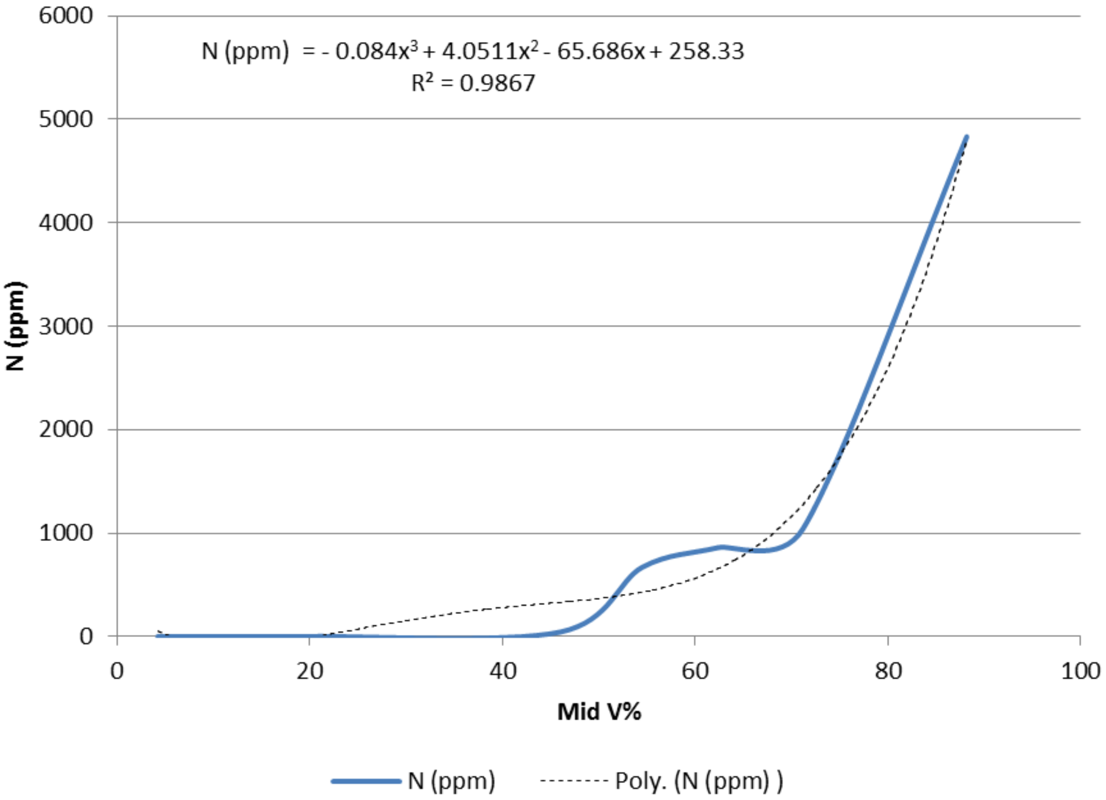


Figure 3.4: N_2 Content Versus Cut Temperature for Arab Heavy Crude Oil

$$N= - 0.084x^3 + 4.0511x^2 - 65.686x + 258.33 \qquad R^2\ 0.9867 \qquad (3.10)$$

Equation (3.10) shows the mathematical form for the arab heavy crude nitrogen content vs cut temperature. For the sulfur content for the heavy Arab crude, as shown in figure 3.5, the model equation can be approximated to a second degree polynomial taking in consideration that higher degree terms can be ignored in this case.

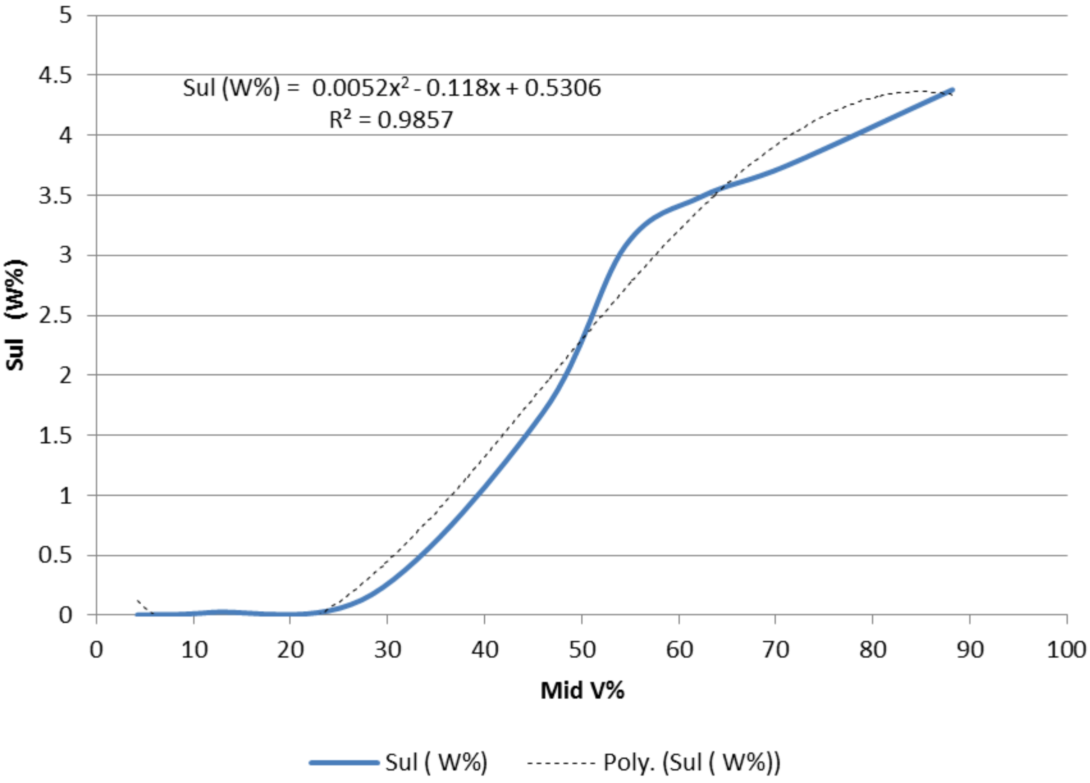


Figure 3.5: Sulfur Content Wt% Versus Cut Temperature for Arab Heavy crude

$$\text{Sul (W\%)} = 0.0052x^2 - 0.118x + 0.5306 \qquad R^2=0.9857 \qquad (3.11)$$

Model Equations for Arab Heavy crude oil:

$$V\% = 0.0004x^2 - 0.0096x - 0.0001 \qquad R^2 = 0.9998 \qquad (3.8)$$

$$API= 0.0444x^2 - 2.5924x + 87.136 \qquad R^2 =0.9989 \qquad (3.9)$$

$$N= 0.084x^3 + 4.0511x^2 - 65.686x + 258.33 \qquad R^2\ 0.9867 \qquad (3.10)$$

$$\text{Sul (W\%)} = 0.0052x^2 - 0.118x + 0.5306 \qquad R^2=0.9857 \qquad (3.11)$$

3.3 Master Model Development

This section describes the overall (master) model that involves all units under consideration in this study. It is written as an optimization problem. The objective function is to maximize profits of selling the final products at the same time, and meet the demand with quality specifications and reduce the NO_X emissions. The main variables are the flows of each stream and products to be processed, intermediate and final products. These include also the properties of each stream such as API, sulphur content, octane number and others. Among the main equations, material balance equations are the most numerous. They usually express the equality between an available quantity of a given intermediate product (product yield at the exit of a unit multiplied by the quantity of feedstock processed) and the quantities used corresponding to the different possible destinations of this product. In this study, a sub-model for each unit, as discussed in the previous section is developed. The model is non-linear since it involves the equations for product properties blending.

The demand equations reflect the fact that the sum of the quantities of intermediate products used in blends to produce a finished product should serve to meet the demand for this product.

Quality equations express the obligation, for each finished product, to meet the legal specification as well as a number of technical requirements. For automotive fuels, these are specific gravity, octane number, sulphur content. For medium distillates and fuel oil legal specifications include specific gravity, sulphur content and cetane number.

The capacity constraint reflects the capacity limitations of existing units. The NO_X emissions constraints require that the overall refinery activity leads to NO_X emissions that are less than current releases within a pre-specified percent level.

The main focus of this study is to provide methods of determining optimal production planning for a petroleum refinery processes. The most important variables will be the feed flow rate, feed properties, products flow rates, and the properties of the products.

The objective is to maximize the total profit of the refinery as follows:

$$profit = \sum_{i \in C} A_i (BP_i) - \sum_{i \in E} B_i f_i - \sum_{i \in I} C_i f_i - \sum_{i \in IF} \sum_{w} D_{i,sw} Z_{i,sw} - \sum_{i \in IF} \sum_{y} E_{i,y} Y_{i,y} \qquad (3.12)$$

The refinery profit is expressed as revenues from selling products minus the costs of purchasing feedstock and costs of operating the process units in the refinery. In equation (3.12) BP_i represents the set of blending units for the final products and their sales price A_i in US$/bbl. The cost B_i (US$/bbl) of the feedstock purchased from external sources is defined under the set (E) for all the units that receive such material from outside. The third term represents the operating cost C_i in (US$/bbl) for each processing unit (i) in the refinery where it is usually expressed as a function of the quantity fed to the running unit. The cost of applying fuel switching is shown in the forth term where Z is a binary variable that represents which fuel (sw) to select. $D_{i,sw}$ (US$/yr) represents the annual cost of switching if fuel (sw) is being chosen. Finally, the profit should be affected by applying NO_X reduction technology, y, with cost $E_{i,y}$ in (US$/yr) if necessary to meet a given NO_X reduction target.

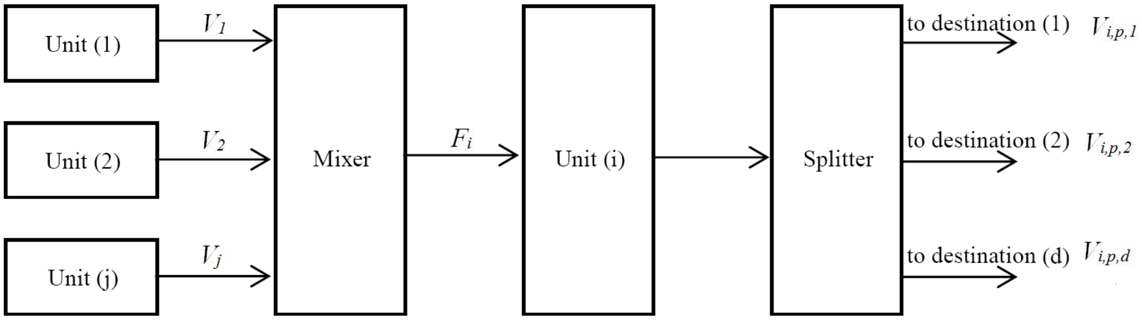


Figure 3.6: Schematic Representation of unit (i) used in the Mathematical Model showing the inlet and outlet streams relations

A general model consists of the following sets of constraints:

- Feed flow rate of processing unit:

$$F_i = \sum_{j \in J} \sum_{p \in N} V_{j,p,i} \qquad \forall i \in I \tag{3.13}$$

The feeds for any processing unit *i* (i belongs to I, the defined set for all the units in the refinery) are represented by F_i is summation of all the possible streams $V_{j,p,i}$ that can be received by unit (*i*) from units (*j*), where (*j*) is defined as the set of all units that can send stream (p) to unit (*i*). Flow rates are in (bbl/yr).

- Feed properties of processing units:

$$X_{i,F} = f\left(V_{j,p,i}, X_{j,p}\right) \qquad \forall i \in I, x \in X_F \tag{3.14}$$

Properties (X_i) of the feed to unit (i) are represented by $X_{\mathrm{i,F}}$ and X_{i} is the set of all feed properties to unit (i). The properties are functions of the streams quantities and properties from unit (j), $V_{\mathrm{j,p,i}}$ and $X_{\mathrm{j,p}}$ respectively.

- Product flow rates of processing units :

$$V_{i,p} = f\left(F_i\,,\, X_{i,F}\,, V_{i,N}\right) \qquad \forall\, i \in I\,, p \in P_i \tag{3.15}$$

Product flow rate from unit (i) for stream (p) is represented by $V_{i,p}$ (p belongs to P the set of all the streams produced from unit i) are functions of the feed quantity F_{i} and property $X_{i,F}$ as well as the operating variables $V_{i,N}$ for unit (i).

- Products properties of processing units:

$$X_{i,p} = f\left(X_{i,F}\,, V_{i,N}\right) \qquad \forall\, i \in I\,, p \in P_i\,, x \in X_i \tag{3.16}$$

$X_{\mathrm{i,p}}$ is the product property (X) for product stream (p) from unit (i) which is a function of feed properties of unit (i) and the operating variables of the unit (i) $X_{\mathrm{i,F}}$ and $V_{\mathrm{i,N}}$ respectively.

- Processing unit capacity:

$$F_i \;\leq\; Umax_i \qquad \forall\, i \in I \tag{3.17}$$

The feed of processing unit (*i*) cannot exceed its maximum capacity, which is represented by $Umax_i$.

The possibility for each product from unit (*i*) to be split to many streams either as final product or feed to other processing unit:

$$V_{i,p} = \sum V_{i,p,d} \qquad \forall i \in I, p \in P_i \tag{3.18}$$

Product stream (*p*) from unit (*i*) is represented by $V_{i,p}$ can be sent to different destinations (*d*) defined by streams $V_{i,p,d}$ (*d* belongs to the set D defined as all the possible units or final products pool that can receive the splitted streams).

- Fuel switching

For each unit i, one fuel should be selected for each furnace of a unit. This constraint is represented by introducing a binary variable $Z_{i,sw}$ that represents the fuel selection (current or new fuel with less NO_X content):

$$\sum_{sw} Z_{i,sw} = 1 \qquad \forall i \in IF \tag{3.19}$$

This means that each unit has to run with a specific fuel, sw. sw is the set of fuels considered.

- NO_X emissions

The annual total NO_X emissions from all units must satisfy a specific NO_X reduction target, $\%NO_X$.

$$\sum_{i \in IF}\left[\left(\sum_{sw} NOx_{i,sw} Z_{i,sw}\right)\left(1-\sum_{y} \varepsilon_{i,y} Y_{i,y}\right)\right] \leq (1-\%NO_x) NO_x \qquad (3.20)$$

In the above equation, the nonlinearity is due to the multiplication of continuous variable $NO_{X\ i,sw}$ and binary variable, $Z_{i,sw}$ and also due to multiplication of two binaries $Z_{i,sw}$ and $Y_{i,y}$.

- Fuel switching or NO_X reduction

For each unit i, if the model choose to switch a specific unit i, no reduction technology will be applied on that unit.

$$\sum_{y} Y_{i,y} + Z_{i,sw} \leq 1 \qquad \forall i \in I \qquad (3.21)$$

- Selection of NO_X reduction process to be installed

This constraint will allow the model select only one reduction process for each unit i belongs to units furnaces set IF.

$$\sum_{y} Y_{i,y} \leq 1 \qquad \forall i \in I \tag{3.22}$$

Equations (3.13) and (3.14) represent the feed quantity and properties of the processing unit model, which are playing an important role on the products flow rates and properties, defined by equation (3.15) and (3.16). Clearly, equations (3.13), (3.17) and (3.18) are linear functions. However, the mixing of the different streams properties coming to the unit as feed, and the calculating of the product flow rates and their properties, equations (3.14), (3.15) and (3.16), are nonlinear functions. All NO_X emissions constraints are non linear.

The developed model for an oil refinery is applied to different case studies in the next chapter.

3.4 Estimation of NO_X Emissions and Products Blending Correlations

This section gives a general procedure for the estimation of NO_X from fuel combustion. Fuel combustion is responsible for about 90% of total NO_X emissions within an oil refinery. Another section is devoted to different blending correlations for refinery final products specifications.

Estimation of NO_X Emissions from Combustion

Fuel combustion NO_X emissions depend upon the amount of fuel consumed and the carbon content of the fuel. To estimate emissions from fuel combustion, the following methodology has been adopted.

NOx emissions = Quantity of fuel combusted x EF per physical unit of fuel

EF is emission factor for a specific fuel. These factors have been obtained and developed from a number of studies conducted by Canada, the United States Environmental Protection Agency (EPA) and other organizations.

Products Blending Correlations

Refinery products are typically the result of blending several components or streams. The purpose of the blending process is to obtain petroleum products from refined components that meet certain quality specification and market demand. Increased operating flexibility and profits result when refinery operations produce basic intermediate streams that can be blended to produce a variety of on-specification finished products. In this study, several blending properties are included in the master model. Blending index for each property is used throughout this thesis. This blending index is reported in the literature for each property. Then, the blending index can be averaged to calculate the blending property value. The following steps are used for that calculation:

First, find index value (n) for each property (X) using appropriate equation. Then find the blending index (b) for each property (X) by the following general equation:

$$b_x = \sum_{p=1}^{P} n_{x,p} w_p \tag{3.23}$$

where b_x represents the blending index for a property X. $n_{x,p}$ is the index for a property X for stream p and w_p is either mass or volume fraction depends on the property. The properties covered in this study are as follows:

API

The density of petroleum oil is expressed in terms of API gravity rather than specific gravity. It is related to specific gravity in such a fashion that an increase in API gravity corresponds to a decrease in specific gravity. The blended API can be calculated by the following equation: (Gary, 1994)

$$API_{blended} = \frac{141.5}{sp.gr_{blended}} - 131.5 \qquad (3.24)$$

Where

$$sp.gr_{blend} = \frac{\sum_{p=1}^{P} RateV_p \times sp.gr_p}{\sum_{p=1}^{P} RateV_p}$$

Where $RateV_p$ is volumetric flow rate of a product stream.

Specific gravity (sp.gr) can be averaged while API cannot.

Sulphur content (wt%)

Sulphur content is an important property which has a major influence on the value of crude oil. The sulphur content for a blended stream is the average sulphur content for all coming streams and should be expressed in weight percent. It can be calculated from the following equation: (Gary, 1994)

$$Sul_{blended} = \frac{\sum_{p=1}^{P} RateW_p \times Sul_p}{\sum_{p=1}^{P} RateW_p} \qquad (3.25)$$

Where $RateW_p$ is the mass flow rate for stream s being blended.

Octane number (ON)

Octane numbers are blended on a volumetric basis using the blending indexes of the components. True octane numbers do not blend linearly and it is necessary to use blending octane numbers in making calculations. Several blending approaches are provided in the literature and the simplest form has been converted to the following analytical relation (Riazi, 2005)

$$N_{RON} = 651X^{3} - 1552.9X^{2} + 1272X - 299.5 \qquad 76 \leq \mathrm{RON} \leq 103 \tag{3.26}$$

Where X = RON/100

$$BI_{blend} = \sum_{p=1}^{P} N_{RON,p} X_{w}$$

Where W_p is the volume fraction and $N_{RON,p}$ is the octane number blending index for product stream p.

Reid Vapour Pressure (RVP)

The RVP is one of the important properties of gasoline and jet fuels and it is used as a criterion for blending products. The Reid vapour pressure is the absolute pressure exerted by a mixture at 100^{o}F (38^{o}C). There are two methods, shown below, for calculating the RVP of a blend when several components with different RVPs are blended. The first method is based on the simple mixing rule using mole fraction (W_p) of each product stream. (Riazi, 2005)

$$RVP_{blend} = \sum_{p=1}^{P} N_{(RVP)p}(w_p) \tag{3.27}$$

Where $(RVP)_p$ is the RVP of stream p in bar or psia.

The second approach is to use blending index for RVP as:

$$(RVPBI)_p = (RVP)_p^{1.25} \tag{3.28}$$

$$(RVPBI)_{blend} = \sum_{p=1}^{P} w_p (RVPBI)_p \tag{3.29}$$

$$(RVP)_{blend} = \left[(RVPBI)_{blend}\right]^{0.8} \tag{3.30}$$

Where $(RVPBI)_p$ is the blending index for $(RVP)_p$ and W_p is the volume fraction of stream p. Both units of bar or psia may be used in the above equation. This relation was originally developed by Chevron and is also recommended in other industrial manuals under Chevron blending number (Riazi, 2005).

Cetane Number and Diesel Index

For diesel engines, the fuel must have a characteristic that favors auto-ignition. The ignition delay period can be evaluated by the fuel characterization factor called cetane number (CN). The behavior of a diesel fuel is measured by comparing its performance with two pure hydrocarbons: n-cetane or n-hexadecane (n-$C_{16}H_{34}$) which is given the number 100 and α-methylnaphthalene which is given the cetane number of 0. A diesel fuel has a cetane number of 60 if it behaves like a binary mixture of 60 vol% cetane and 40 vol% α-methylnaphthalene. Another characteristic of diesel fuels is called diesel index (DI) defined as:

$$DI = \frac{(API)(1.8API + 32)}{100} \qquad \text{(Riazi, 2005)} \qquad (3.31)$$

which is a function of API gravity and aniline point (AN) in ^{o}C. Products containing aromatics or naphthenes have lower aniline points than products containing paraffins. Cetane index (CI) is empirically correlated to DI and API in the following form:

$$CI = 0.72DI+10 \qquad (3.32)$$

It is reported in the literature that cetane number can be blended by volume basis (Baird, 1987) as in the case of specific gravity.

Smoke point

Smoke point is a characterization of aviation turbine fuels and kerosene and indicates the tendency of a fuel to burn with a smoky flame. Higher amount of aromatics in a fuel causes a smoky characteristic for the flame and energy loss due to thermal radiation. The equation to calculate the smoke point index is (Riazi, 2005):

$$IN_{SP} = \frac{1}{SP} \tag{3.33}$$

The methodology of finding the blended smoke point is via the blending index and then by applying equation (3.31).

The previous blending correlations are implemented into the model for finding final product specifications.

Chapter 4

Results and Discussion

4.1 Introduction

The mathematical model developed in chapter three for oil refinery is illustrated for different case studies. The new contribution in this work in comparisson to the original model is the modeling of the CDU for heavy light crude oil and the addition of the viscobreaker unit into the mathematical model. The endorsed mathematical model is an extension of the previously applied model which was superstructed by Ba-Shammakh (2010). However, in this model, the viscobreaker effect is covered and investigated throughly. The viscobreaker has been used in many oil refineries for a long time. However, the viscobreaker unit was not included in any of the previous mathematical models of oil refinery profit optimization. In addition, the NO_X pollutant reduction from oil refinery has never been considered in previous studies for finding the optimal profits. NO_X regulations are enforced into refinery has sector in USA and Canada. The cost due to removing of NO_X from the plants is essentially must be included in our cost table since it can potentially come at premium.

In this work, the subject of NO_X reduction is investigated using different techniques. There are many ways in reducing the NO_X emissions. In order to decide how to make the NO_X reduction for a specific unit in the refinery, we need substantial input data before setting anything conclusively. Equally it is important to include NO_X reduction data in the mathematical model which will do the work to reach an optimal value for profits and simultaneously meet other constraints.

There are two fundamental reasons for including NO_X reduction into the refinery mathematical model. First, the cost of NO_X reduction is very high and it becomes a regulation that must be strictly followed in many countries all over the world. Secondly, there are several ways in reducing the NO_X from refinery and each method of NO_X reduction has its own limitations and expense. Since the industry's interest is profitable acquistions and reducing the losses, it is imperative to construct a mathematical model that considers these two factors: cost and limitation, abling to make a feasible solution with maximum profits. Inderterminately one must utilize the GAMS software in calculating the most economic approach in reducing NO_X for a specific unit from the refinery to a specific level discerning the amount of NO_X removed. The options considered here for the NO_X reduction are the followings:

1. Balancing:

   In which the production from units that emit less NO_X is increased with decrease in the production from units that produce more NO_X during the heating process. This is accurate because fuel burning for each unit is a function of inlet flow rate.

2. Switching:

   In which the unit will be switched to operate with less NO_X content fuel.

3. Applying NO_X reduction technologies:

Many technologies for NO_X reduction are very common in industry and they vary in operating and maintenance costs. However, they are very effective and can remove more NO_X than balancing and switching techniques.

The results for various case studies are given at the end of this chapter. The cases under study are:

- Case A: Planning model (base case) without any NO_X reduction target.
- Case B: Planning model with all three mitigation options mentioned above (with NO_X reduction).

4.2 Problem Description for Case Studies

Profitable operation of a refinery requires an optimization of streams flows and process feed. Notwithstanding, several trends in the oil refinery industry are leading to a compact production of different products because of new specifications and environmental regulations. The increased market for heavier crude oils force refineries to increase their use of conversion units. Hydrocracking and viscobreaking, as conversion units, are ways of upgrading heavy oils to more valuable products. More hydrocracking and viscobreaking, in addition to the other units in the refinery, results in more burning which leads to more NO_X emissions to the air. The major source of NO_X emission within an oil refinery is combustion source such as furnaces. An efficient model for the refinery planning will represent production planning with different NO_X mitigation options in order to meet a certain NO_X emissions reduction. The model is illustrated for different case studies. The objective in the model is to maximize the profit of an oil refinery by producing certain amount of each product with specific quality and meet NO_X reduction target by implementing several mitigation options. The options being considered in this study, as mentioned earlier, are flow rate balancing, fuel switching and application of NO_X reduction technology such as SCR.

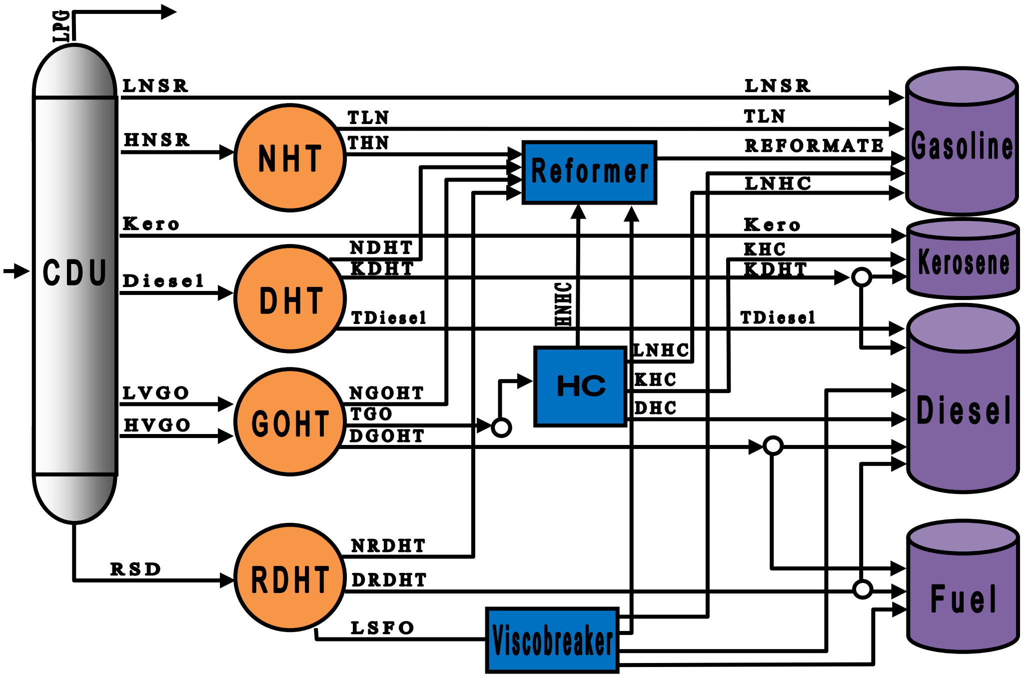


Figure 4.1: Oil Refinery layout showing all main process units

The oil refinery shown in figure 4.1 consists of several processing units, splitters and mixers. The connections between these units, splitters and mixers draw the refinery network picture that general model aim to solve in meeting the objective of model planning. Refinery intermediate streams with different properties are blended in order to feed a processing unit or to be ready for sale as a final product. For both cases (Case A and B), the blended streams must meet a degree of required specifications. Nonlinear models describe more accurately product flow rates and properties than linear models assuming fixed yield. Non linear models are presented and linked with nonlinear properties blending equations in order to build the over all Model. The overall model is integrated with a NO_X management model in order to reduce NOx emission from combustion source within an oil refinery. The aim of the model is to optimize the flow rate and properties for each stream in order to maximize profit while reducing NO_X emissions to a given target. The optimization quandary being studied in this chapter is stated:

“For a given NO_X reduction target, what is the best strategy or mix of strategies, for an oil refinery, among the considered options (flow rate balancing, fuel switching and NO_X reduction technology) in order to meet the demand for each product with quality specifications while maximizing the profit?”. The objective is to maximize the profit of selling the final products to meet the demand with quality specifications and reduce the NO_X emissions to a given level. The main variables are the flows of each stream and products to be processed, intermediate products and finished products. These include also the properties of each stream such as API, sulphur content, octane number, RVP, cetane number and smoke point. A binary variable, Z, is introduced into the model that represents fuel switching. Also another binary variable, Y shows whether NO_X reduction technology has been applied.

Individual nonlinear mathematical models (sub-models) were developed for the CDU and viscobreaker units, shown in figure 4.1, prior to the development of the planning model. The sub-models were developed for: the crude distillation unit (CDU), all the hydrotreaters, the reformer, viscobreaker and the HC. Visebreaker modeling is the additional work done under this study to the original model developed by B-Shammakh (2010).

The model is formulated as an MINLP since nonlinearity is present from the blending correlations and the binary variables introduced for the switching and NO_X reduction options.

Three different options are considered as discussed earlier:

- Option 1: Flow rate balancing
- Option 2: Fuel switching
- Option 3: Existence of NO_X reduction technology

Fuel switching represents switching from current fuel to some new fuel with less NOx emissions. The NO_X reduction process used in this study is SCR which is Selective Catalytic Reduction.

The model developed in chapter 3 is solved in this chapter and is applied to different case studies.

4.3 Results and Discussion

4.3.1 Analysis of Visbreaker Converting crude to Final Products:

As mentioned earlier, viscobreaker unit contribution into the optimization of oil refinery has never been considered in previous studies. In order to see how effective the viscobreaker, we will examine more details about the viscobreaker using some known formulas. Figure 4.2 shows the inlet and outlet streams from the viscobreaker unit considered in an oil refinery.

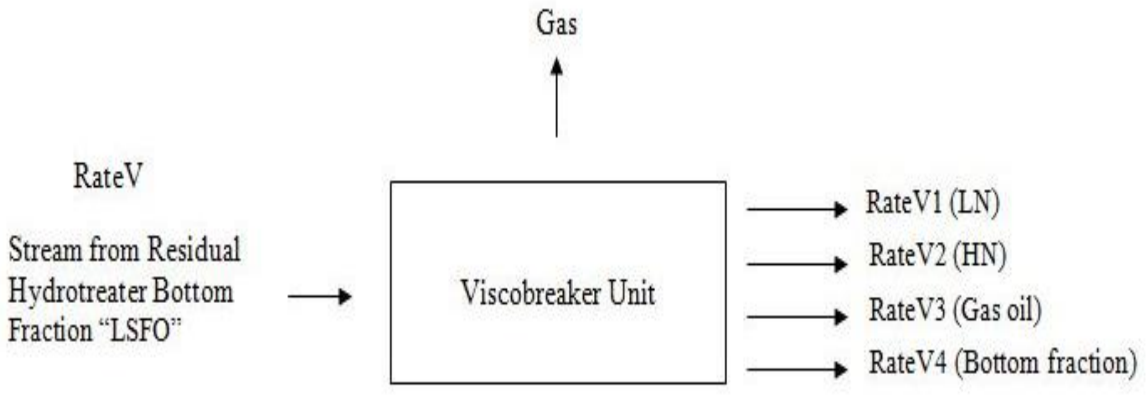


Figure 4.2: Viscobreaker Inlet and Outlet Streams

When connecting the viscobreaker to our mathematical model, the feed to the viscobreaker is coming from the outgoing stream from the bottom fraction for CDU residual hydrotreater. The CDU residual hydrotreater line is shown in figure 4.1 as "LSFO" stream (Light Straight Fuel Oil). This "LSFO" stream is extremely heavy crude oil and it is coming from residual hydrotreater bottom fraction. However, through the viscobreaker, the extremely heavy materials can be converted to product that can be sold as gasoline, diesel and naphtha. The viscobreaker through extreme heating can convert the residual hydrotreater bottoms to light naphtha, heavy naphtha, gas oil, and heavy bottoms. The streams are discussed in details below to show the contribution from visbreaker to the mathematical model. The feed stream "RateV" and "LSFO" stream from figure 4.2 are both in volume unit of (bbl). Since original viscobreaker formulas are in mass units, we need to convert to volume units to be consistent with the remaining model units. Below is the formula used to convert the volume to mass in (KIb).

Mass (KIb) = Volume (BBL) x (SG) x (.3502)

SG = Specific gravity of the stream

The above equation is already implemented in the model. Table 4.1 shows the outlet stream products from viscobreaker unit in volume unit of BBL.

Table 4.1: Visbreaker Inlet and Outlet Streams

Stream	**Description**	**Amount (in BBl)**
RateV (feed to viscobreaker)	Feed stream to viscobreaker	53,399 bbl
RateV1 (outlet stream)	Light Naphtha	54 bbl
RateV2 (outlet stream)	Heavy Naphtha	113 bbl
RateV3 (outlet stream)	Gas oil	163 bbl
RateV4 (outlet stream)	Bottom fraction	18,229 bbl

The light naphtha stream from viscobreaker is sent to the gasoline pool directly as shown in figure 4.1. The second stream, heavy naphtha is sent to the reformer then from the reformer it is sent to the gasoline pool. The third stream from viscobreaker, gas oil stream, is sent to the diesel pool. The fourth and last stream is the heavy bottoms which are sent to the fuel oil pool. The selected destination of the outlet streams from the viscobreaker is based on its cut temperature. For example, the light naphtha stream cut temperature range is 0-180 ^{o}C. Similarly, other streams are distributed according to their cut temperatures. From table 4.2, we can see that per 100,000 barrels of crude processed on a daily basis, the viscobreaker can produce 19,170 barrels/year of light naphtha, 41,248 bbl/year of heavy naphtha, 59,495 bbl/year of gas oil and 6,655,000 bbl/year of heavy bottoms (asphalt materials). The numbers mentioned so far indicate the power of viscobreaker as a processing unit in the refinery. We need to emphasize that the products from visbreaker are based on 100,000 of crude oil processed on a daily basis. There are many refineries around the world that can produce double or triple this amount. That indicates that the products stream from the viscobreaker and profits related to these products can be double or triple the amounts mentoned in table 4.2.

Table 4.2 shows the products streams from viscobreaker unit on a basis of 100,000 crude oil processed on a daily basis including the annual total sales in dollars for each product.

Table 4.2: Visbreaker product streams with total sales on yearly basis.

Stream #	**Description**	**Volume in (bbl/year) produced**	**Total sales per year ($)**
1	Light Naphtha	19, 710	2, 128, 680
2	Heavy Naphtha	41, 248	4, 455, 000
3	Gas oil	59, 495	7, 140, 000
4	Bottom Fraction	6,655,000	439, 000,000

However, without the viscobreaker being included in the model, the total bottom fraction from residual hydro treater will be sold as fuel oil or asphalts. Table 4.3 below shows a comparison of sales with and without considering the viscobreaker. Table 4.3 shows the effect of including the viscobreaker unit in the model of oil refinery to the refinery profits.

Table 4.3: Comparison for Sales with and without Viscobreaker

Total sales per year without considering the viscobreaker ($)	**Total sales per year considering the viscobreaker ($)**
370,961,910	452,859,000

The difference between the total sales mentioned in the above table is estimately $82,000,000 annually. Signifying with considering the viscobreaker in the refinery model, the refinery profits can increase by $82,000,000 every year assuming that we are processing 100,000 barrels of crude per day. Now, we can conclude that it is extremely important for oil refinery planning model to include the viscobreaker products since it will, in addition to the extra significant profits, contribute in a significant amount to increasing production of gasoline, diesel and fuel oil. Resultantly, we discuss the two cases with and without NO_X reduction.

4.4 Mathematical Model with NO_X Reduction (Case A & Case B):

The two cases we are discussing in our model are case A & case B as described earlier.

Case A: Solve the planning model to meet demand and specifications without any NO_X mitigation option which means 0% of NO_X reduction requirement.

Case B: Solve the planning model with quality constraints considering flow rate balancing, fuel switching and NO_X reduction technology. The model is a MINLP.

In order to illustrate the model, figure 4.1 for a petroleum refinery process is used. A 100,000 bbl/day arab heavy crude oil is selected to be the feed to the refinery. The refinery has to meet the market demands for different products which are shown in table 4.4. The product price is given in the same table. The product prices are based on USA market in 2011. Also, product specifications have to be met as shown in table 4.5 in addition to a certain NO_X emissions reduction target. The results are based on 100,000 bbl/day of crude oil processed. However, most major refineries are producing above this number. For example, in Saudi Arabia, Ras Tanura Refinery is processing around 250,000 bbl a day.

Case A is the case without considering the removal of NO_X. Case B is the case where we start NO_X reduction and hypothesize how this reduction will affect the total profits. Table 4.4, lists the four main products from refinery and these are the Gasoline, Kerosene, Diesel and Fuel oil. The demand assumed in this study is 20,000 bbl a day for all products except for the fuel oil which is assumed to be 18,000 bbl/day. The basis of my assumption is to make the model as simplistic as possible from demand point of view because the purpose of this study is to look after the NO_X reduction analysis and profits changes. However, the mathematical model is flexible for changing the demand in order to look for different cases with different demand values. The prices shown for the four products in table 4.4 are in $/bbl as per USA market average price of March 2011. As seen in table 4.4, diesel has the highest price value among other products with $120/bbl. This is because diesel has higher demand than other products. The lowest price product is the fuel oil with 66$/bbl since it has the lowest demand. Looking at the product prices one can say that the result of the optimized mathematical model should reflect more diesel than other products since the demand of all main three products are the same. As mentioned, the prices of the four products are based on average USA local market prices.

Looking at table 4.5, listed are the main properties of the four products which must be met. The mentioned properties are added as constraints in the mathematical model. Meaning the properties must be satisfied in all cases to reach an optimal solution. For example, from table 4.5 we can read that the specific gravity, S.G., for gasoline should not exceed 0.817. In the mathematical model it is been added as a constraint that the SG for gasoline should not exceed that value. Table 4.5 is showing all other properties constraints which have been added to our mathematical model. These constraints originate from international and oil industry standards to comply with high quality of the four products before they are sent to sale. Therefore, these properties are included into the mathematical model as constraints.

Table 4.4: Products demand

Final Product	**Demand bbl/day**	**Price US$/bbl**
Gasoline	20,000	108
Kerosene (Jet Fuel)	20,000	86
Diesel	20,000	120
Fuel Oil	18,000	66

The objective function will be to maximize the overall refinery revenue while meeting market demand, quantity and quality with certain NO_X reduction target. Meeting the quality demand includes meeting all properties constraints in table 4.5. This will make a powerful tool of this model for future plans in the refinery. It can also predict whether we can meet a specific constraint, standard or requirements. The model is a complicated program that can operate for several changes of properties simultaneously. However, it is very sensitive to changes. For example, it may not reach an optimal value due to small changes in S.G. for any of the products. However, this can be solved sometimes by changing the upper limit of the S.G. of that product.

Table 4.5: Products specification

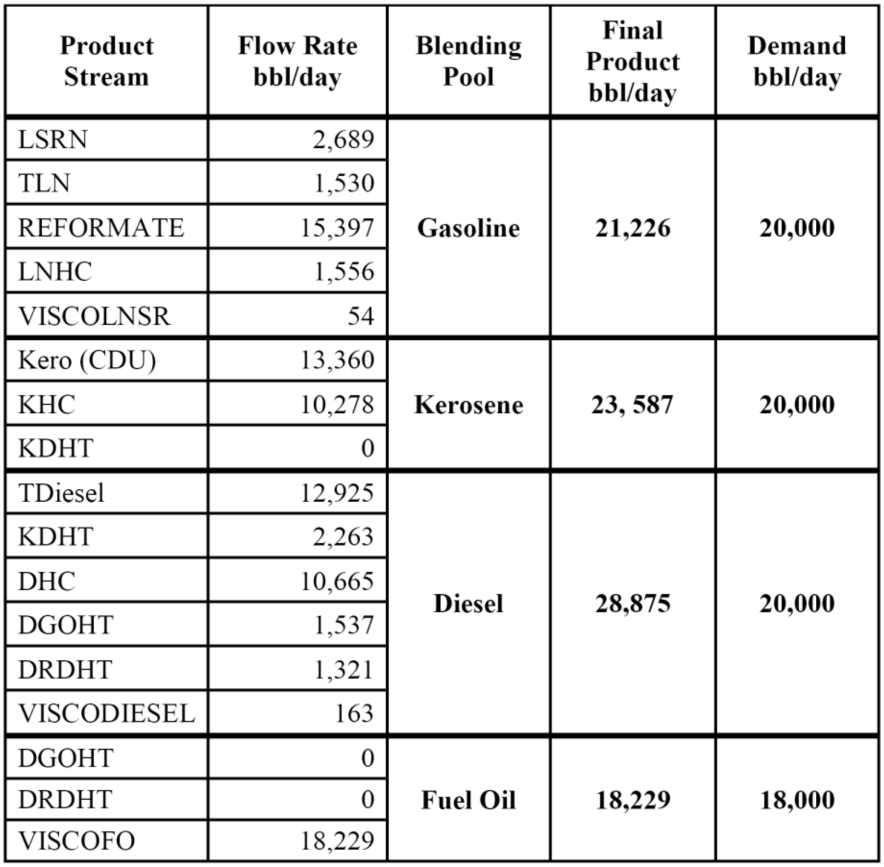
Final Product	**Property**	**Specification requirement**
Gasoline	S.Gr	≤0.817
	Sul%	≤0.05
	RON	≥89.0
	RVP, psi	≤9.0
Jet Fuel	S.Gr	≤0.85
	Sul%	≤0.25
	Smoke Point	≥20.0
Diesel	S.Gr	≤0.875
	Sul%	≤0.5
	CN	≥45
Fuel Oil	S.Gr	≤1.0
	Sul%	≤1.0

The model was coded into the General Algebraic Modeling System (GAMS). The GAMS model optimizes all intermediate and final products streams across a crude oil refinery subject to connectivity, capacity, demand, and quality constraints with certain NO_X reduction target. These constraints can be easily modified to incorporate new data. Now we will be discussing the two cases mentioned earlier (Cases A&B).

Case A: The model is solved and considered as our base case for comparison purposes later. NLP is the model technique used for the planning. A summary of every blending pool streams flow rate for Case A (without NO_X reduction target) is illustrated in table 4.6 with a total profit of $7.25x10^8$ \$/yr including satisfying other constraints with total NO_X emissions of 10,636 tonne/yr. That means the refinery is producing a total of 10,636 ton of NO_X every year which will go directly into the air. It is really huge amount of air pollutant and needs to be reduced. We will see later how we will reduce the NO_X and its relation to the refinery profits. Table 4.7 shows the product properties that the model is trying to satisfy while meeting the demand. The last column represents the model results.

It is clear from the two tables that the planning model tries to meet the demand requirement for each product and the properties required for meeting the quality constraint for each final product. The most profitable product among an oil refinery is diesel. So, the model tends to produce more diesels while meeting the demand for other products is also mandatory. The model suggests that the diesel production is 28,875 bbl for every 100,000 bbl of crude oil processed. Ranking the diesel as the highest in final product, kerosene comes next with 23,587 bbl. We can see that although kerosene price is cheaper than gasoline, but still the model suggest producing more kerosene than gasoline. Gasoline volume produced per 100,000 bbl of crude is 21,226 bbl which is less than kerosene by around 2000 bbl. We can conclude that the model is considering other factors in addition to the price of the product. These factors are the required specification of final products which are shown in table 4.5.

Table 4.6: Blending products flow rate



Product Stream	**Flow Rate bbl/day**	**Blending Pool**	**Final Product bbl/day**	**Demand bbl/day**
LSRN	2,689	**Gasoline**	**21,226**	**20,000**
TLN	1,530			
REFORMATE	15,397			
LNHC	1,556			
VISCOLNSR	54			
Kero (CDU)	13,360	**Kerosene**	**23, 587**	**20,000**
KHC	10,278			
KDHT	0			
TDiesel	12,925	**Diesel**	**28,875**	**20,000**
KDHT	2,263			
DHC	10,665			
DGOHT	1,537			
DRDHT	1,321			
VISCODIESEL	163			
DGOHT	0	**Fuel Oil**	**18,229**	**18,000**
DRDHT	0			
VISCOFO	18,229			

Table 4.7: Product properties after running the model

Final Product	Property	Specification requirement	Model
Gasoline	S.Gr	≤0.817	0.816
	Sul%	≤0.05	0.000416
	RON	≥89.0	92.129
	RVP, psi	≤9.0	7.409
Jet Fuel	S.Gr	≤0.85	0.834
	Sul%	≤0.25	0.199
	Smoke Point	≥20.0	21.38
Diesel	S.Gr	≤0.87	0.852
	Sul%	≤0.5	0.044
	CN	≥45	55.334
Fuel Oil	S.Gr	≤1.0	0.865
	Sul%	≤1.0	0.201

There are three split points that we need to discuss here in order to show how the model can selectively send their products. As we said earlier, we tried to simplify the model as possible in order to make it easier to understand and be able to visualize the power of the results more clearly. Looking at the first split point, stream “KDHT” coming from unit “DHT” as shown in figure 4.1, the stream “KDHT” will split to the diesel pool and the jet fuel pool. However, reconnoitering model result, it showed that the “KDHT” stream product, which is about 2263 bbl, is contributing to the diesel pool. The model decided to send zero product to the jet fuel pool at the split point since the diesel price is higher than jet fuel price. The model decision is based on the fact that the model objective function is to maximize the profit while keeping other constraints satisfied. The second split point is at the “DGOHT” stream which is emanates from the “GOHT” unit as shown in figure 4.1. The “DGOHT” stream is splitted between the diesel pool and the fuel oil pool. The model result, as shown in table 4.6, is sending the total product, around 1537 bbl, to the diesel pool while sending zero products to the fuel oil pool. Suitably, since the demand and other constraints are satisfied, the model tries to keep the objective function magnified by maximizing the profits. Inasmuch the model decided to send the entire “DGOHT” stream product to the diesel pool. Similarly, the “DRDHT” stream ensuing the “RDHT” unit is splitted between the diesel pool and the fuel oil pool. At the split point the model needs to make a decision on where to send the stream.

It will send the product to either the diesel pool or the fuel oil pool. The model suggests sending these products, which is around 1321 bbl, to the diesel pool instead of the fuel oil. As seen from table 4.6, the total product amount of 1321 bbl is sent at the split point to the diesel pool in order to maximize the objective function which represents the profits. This demonstrates the satisfactions of all specifications mentioned in table 4.5 while sending all products at the three split point to the diesel pool. If we could lower the demand for the fuel oil (or if it could be met by other intermediate products) the model will try to produce more diesels. This would be expected, when lowering the fuel oil demand, because the diesel has the highest price in the market. The model will tend to increase the profits as possible by increasing the diesel product. However, this will be done after satisfying the new lower demand of the fuel oil.

As noticed from the tables above for case A (with no NO_X reduction), the model result has met all properties specification and requirement. One Primary example is when the goal of diesel properties are being met. The specific gravity is near the desired value with 0.852 as the model result versus 0.87 as the maximum specification allowed for diesel S.G. The difference is only 0.018 which indicates that the model is giving a very good value for the diesel S.G. For the diesel sulphur content we got from the model result a value of 0.044% versus 0.5% as the maximum allowed in the specification of diesel with sulphur content much lower than the specified range by 0.456%. The model aims to minimize the sulphur content as much as possible. The cetane number for the diesel should not be less than 45 as mentioned in the diesel specification. The model result for the CN was 55.33 which is above the specification limit by 10.33. This shows that our CN for the diesel is the safe side in terms of meeting product specification. The model tries to maximize the CN as much as possible while keeping other properties in the safe range.

The properties for jet fuel are tighter than those for gasoline and they are all near the limit. For jet fuel, the specifications call for a maximum of 0.85 for the S.G and the model result was 0.834 with a difference of 0.016 only. However, it is still in the safe range. For the sulphur content of jet fuel, the model result was 0.199% versus 0.25% as the maximum allowed per specifications with a difference of 0.051% showing lower value sulphur content than the specified one. The model showed 21.380 for the smoke point of jet fuel which is higher than the specified minimum of 20.0. For gasoline, all properties are met. For example, SG is very near to the specified value. The model showed a value of 0.816 for the S.G of gasoline while the specification is requiring an upper limit of 0.817 with a safe difference of 0.001. The sulphur content of gasoline as per the model result showed 0.000416 where the specifications are giving a limit of up to 0.05. The RON of gasoline for the model result was 92 while the specification is giving a lower limit of 89. The fuel oil property constraints are all satisfied with specific gravity constraint as the only binding one. The fuel oil S.G from the model result was 0.865 where the specifications upper limit is 1.0 showing an extremely acceptable difference. The sulphur content of fuel oil from the model output was 0.21 which is way lower than the specifications by around 0.8. Now we will investigate the NO_X mitigation cases starting with base case (Case A).

Figure 4.3 illustrates the NO_X emissions from each unit (combustion source) without any mitigation options (Case A). The fuel used in combustion for all units is assumed to be fuel #6. The profit is 7.25×10^8 \$/yr with total NO_X emission of 10,638 ton/yr.

This case will be used later for comparison with other NO_X reduction cases to study and analyze the cost effect with NO_X reduction percentage. From figure 4.3, we noticed that CDU is producing 2929 ton/yr of NO_X, reformer is producing 1980 ton/yr of NO_X and GOHT (gas oil hydro treater) is producing 1895 ton/yr of NO_X. This indicates that around 64% of total NO_X produced from the eight refinery units is coming from the CDU, reformer & GOHT units. These units are sharing the major part of the pollutant mass.

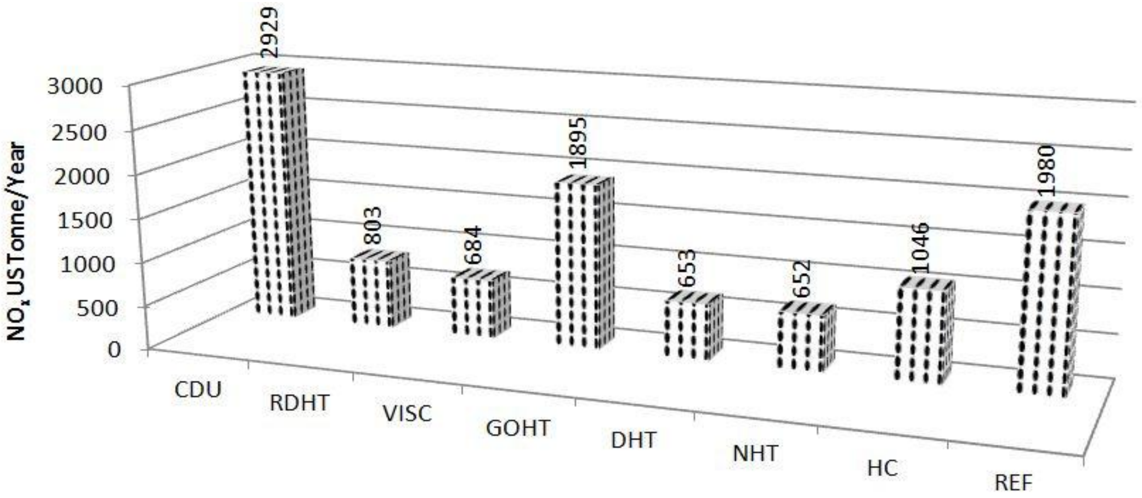


Figure 4.3: Case with total emission from all units

In the other hand, the NHT, DHT, Visc, HC and RDHT are the less producing units of $NO_{X.}$ The five units are responsible for around 36% only of the total pollutant produced every year. Figure 4.3 is giving us a good idea about where the major pollutant is coming from. Next, we will be studying how to reduce the NO_X, how much will be reduced and what is the optimal method for NO_X reduction for each unit. Figure 4.3 will be used along with other reduction targets for comparsion to the changes happending at each reduction target.

Case B:

Planning model with quality constraints and NO_X mitigation by balancing, fuel switching and application of NO_X reduction technology are considered in this case study. The NO_X reducing process under consideration is SCR process since it is commercially available at large scale. The cost for NO_X reducing process is implemented in the model. A binary variable, $Y_{i,k}$, is introduced in the model to find whether NO_X reducing process is used in unit and what technology is being used. The binary variable will show whether a certain technology is being used. Another binary variable, $Z_{i,SW}$ is introduced to indicate whether current fuel or new fuel is being used to help us know about the second mitigation option which is the fuel switching. If fuel switching option is applied, the binary variable $Z_{i,SW}$ will have a value of 1. If the switching is applied, the model will tell us what fuel to switch to. In our case here, we have one new fuel. So, when switching is applied, it means the model is switching to the new fuel. Also, the mathematical model will not allow both of fuel switching and SCR technology to be used at the same refinery unit. There is a conditional equation that controls this situation of not allowing both of the SCR application and fuel switching to be selected for the same unit.

Table 4.8: Emission factors for the three NO_x mitigation options

Option	Emission Factor
Fuel #6 (Current or old Fuel)	1.04
Fuel #2 (Proposed New Fuel)	.46
SCR Technology	.104

Looking at the table above, it is evident how the three options of current fuel, new fuel and the use of SCR technology vary in terms of their power to reduce NO_X emissions for refinery units. Since NO_X is a function of the fuel required for heating the inlet stream, NO_X is also a function of the feed to the refinery unit. The more feed comes into the oil refinery unit, the more fuel you need for heating. However, same amount of current fuel and new fuel produces different amount of NO_X. New fuel produces less NO_X than current fuel. However, only at low NO_X reduction target, new fuel can help. The emission factor for SCR technology was calculated based on the fact that SCR can remove 90% of NO_X produced by current fuel. Hence, by multiplying the emission factor for current fuel by 0.9, we the obtain SCR technology emission factor.

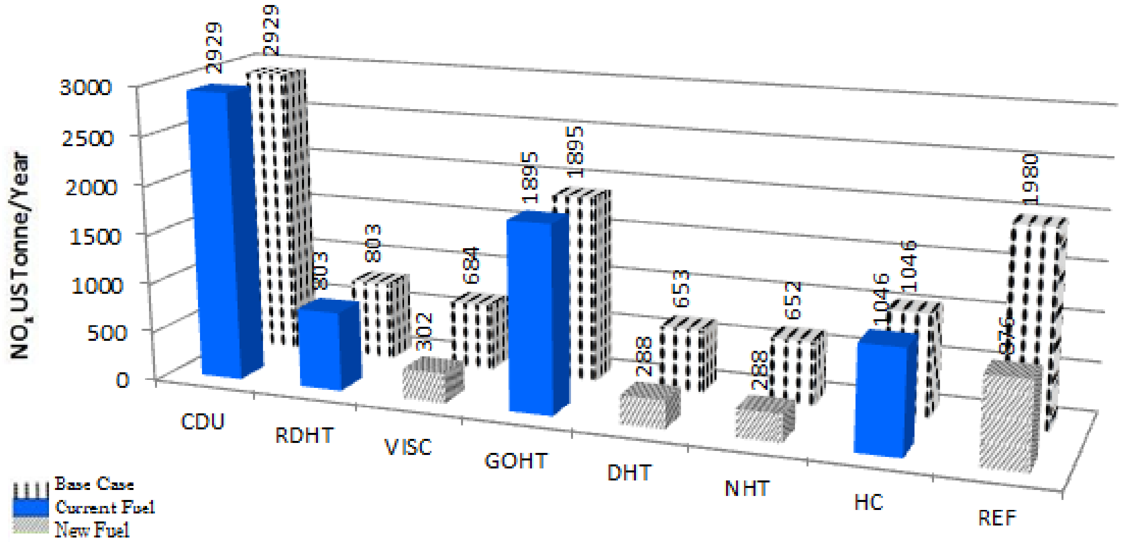


Figure 4.4: Case with 20% Reduction in NO_X

By looking at figure 4.4, for 20% reduction target, we notice no SCR is implemented. Since the mathematical model can achieve the target of 20% NO_X reduction without the need for implementing a high cost technology, it will automatically choose to switch to new fuel. For 20% NO_X reduction, the model chose to switch only four units to new fuel (Viscobreaker, DHT, NHT & Ref.). We can see that three is around 50% reduction in NO_X emission from each of these units. The remaining units stayed with current (old) fuel. It means one can obtain 20% reduction of total NO_X from the refinery by reducing around 50% of NO_X emissions for each of the four mentioned units. As we noticed for the 20% reduction target, the model selected mostly the units with small to medium size in terms of NO_X production.

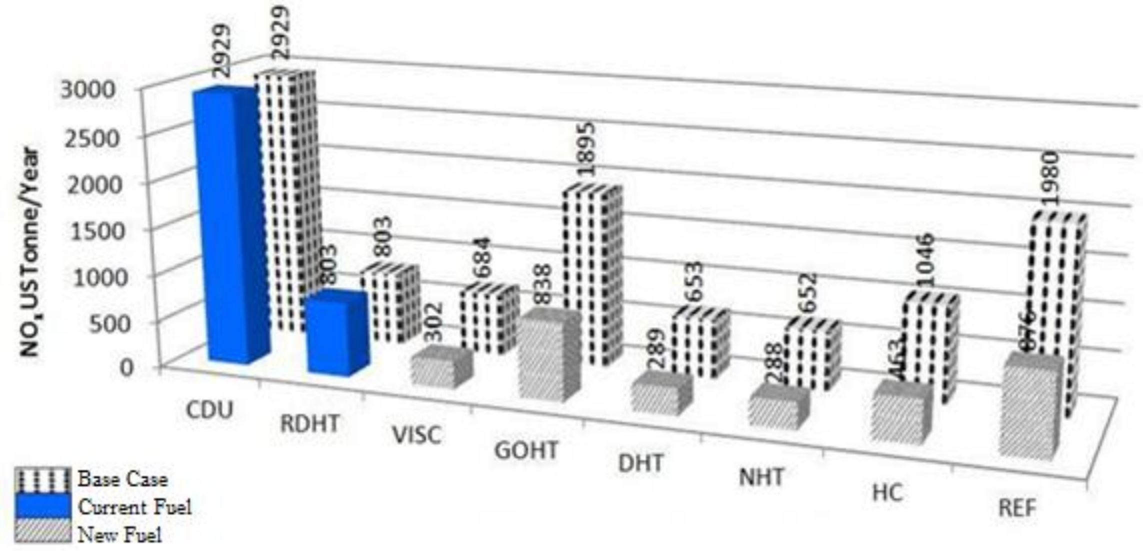


Figure 4.5: Case with 40% Reduction in NO_X

Figure 4.5 shows the results for 40% NO_X reduction. The model chose to switch six units (VISC, DHT, NHT, GOHT, HC and REF) to new fuel. Note that not all units have been switched to new fuel. Two units kept running with current (old) fuel. These units are CDU and RDHT. The differences are only in the number of switched units and in the resulting profit which decreases as NO_X reduction target increases. The base case (Case A) is shown in each figure for easy comparison. As noticed, for the case of 40% NO_X reduction, more units switched to new fuel than in the case of 20% NO_X reduction. However, when 40% of NO_X is required, the model switched more units to new fuel. Looking again at figures 4.4 & 4.5, we notice that the same fours units for the 20% and 40% reduction were switched to new fuel with the same amount of reduction. However, for the 40% reduction, two more new units were affected by fuel switching and these are the GOHT & HC units. Both of these units were reduced by around 60% for each in order to reach the target of 40% total reduction of the refienry. That means switching the six units to new fuel (four units reduced by 50% and two units reduced by 60%), can achieve the target of 40% reduction of total NO_X. We can conclude that for the 40% reduction target six units have been switched to new fuel. Even at the 40% NO_X reduction target, the model tried to avoid using the SCR technology as much as possible since the main target is to maximize profits and reduces losses by avoiding unnecessary additional cost of SCR technology.

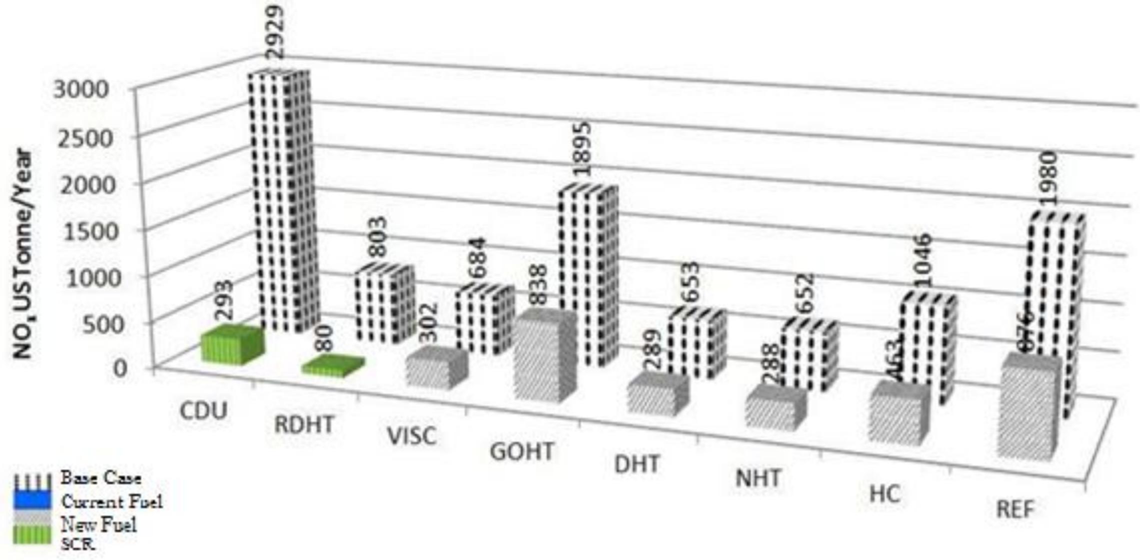


Figure 4.6: Case with 60% Reduction in NO_X

For higher reduction targets, such as 60% (see Figure 4.6), more NO_X needs to be removed from more units. The model chose to remove NO_X by the SCR technology from two different units. These units are CDU, RDHT. These units have the highest impacts on the overall NO_X emission. These two units never have been subject for reduction by the model for the previous 20% and 40% reduction target cases. Six units are chosen to be switched to new fuel and these units are GOHT, NHT, VISC, HC, DHT and REF. These units are reduced in a similar way to what the model did for the 40% reduction target, see figure 4.5. At the 60% reduction, we see a combination of SCR and new fuel options in the refinery. The model decided to switch some units to SCR technology and other units to new fuel option. Insofar, the model targeting is less use of SCR in reducing the total cost. It is seen that SCR technology was used for the removal of NO_X from two units which have major emissions of NO_X. The model tries to minimize the use of SCR technology as more NO_X removal will increase the operational and maintenance cost of the SCR technology. But always remember that SCR can remove up to 90% of NO_X produced by a refinery unit. The model tried to do a good balancing between the technology use (SCR) and the switching to the new fuel while maintaining the required reduction target of 60%.

Figure 4.7 shows the result for 80% reduction target. The results show that NO_X emissions should be removed by SCR from four units and only NHT, REF,VISC units have to be switched to new fuel as was done for the 60% reduction. Four units will be using the SCR technology to remove NO_X and these are the CDU, RDHT, GOHT and HC. The CDU & RDHT units are similar to the 60% reduction case where the SCR technology was used. However, we see that one unit which is the DHT is remaining with the current fuel and it was not subject to switching or applying of technology. This is done to achieve the reduction target and maximize the profit. However, it is found that 90% is the maximum possible reduction target when all NO_X emissions from all units are removed by SCR. A summary of results for case A and B with NO_X reduction is given in table 4.9. It shows that the profit decreases by about 1.5% at 40% NO_X reduction target.

About 3.28% drop in profit noticeably at 80% NO_X reduction when NO_X emissions from seven units are removed.

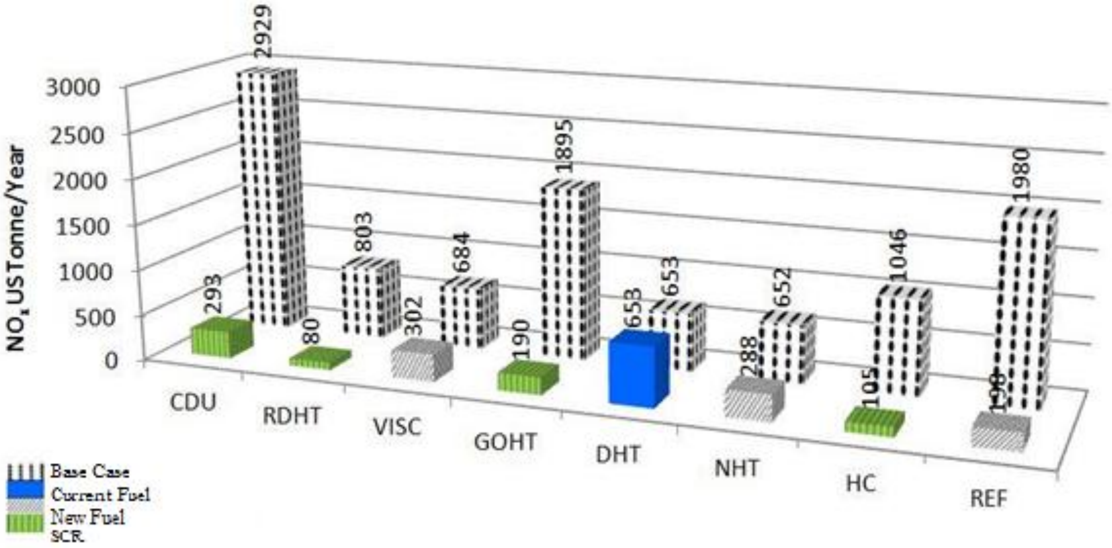


Figure 4.7: Cases with 80% Reduction in NO_X

Table 4.9: Summary of Results for Variation in NO_X Reduction and Profit Change

% Reduction	**Profit (million $/yr)**	**NO_X emission (Ktonne/yr)**	**% Reduction in Profit**
Base Case	725.3	733.0	0
20	720.8	440	0.62 %
40	714.7	293	1.5 %
60	708.2	147	2.36 %
80	701.5	73.3	3.28 %

Figure 4.8 shows the profit for each reduction target for this case study. Figure 4.8 shows a semi linear relationship between profits and NO_X reduction percentage target. Almost the profits drop by about 0.041% for each one percentage increase in NO_X reduction percentage target. The profit decreases as more NO_X emissions are removed from more units. By looking at figure 4.8, we can predict our profits drop when increasing the NO_X reduction target.

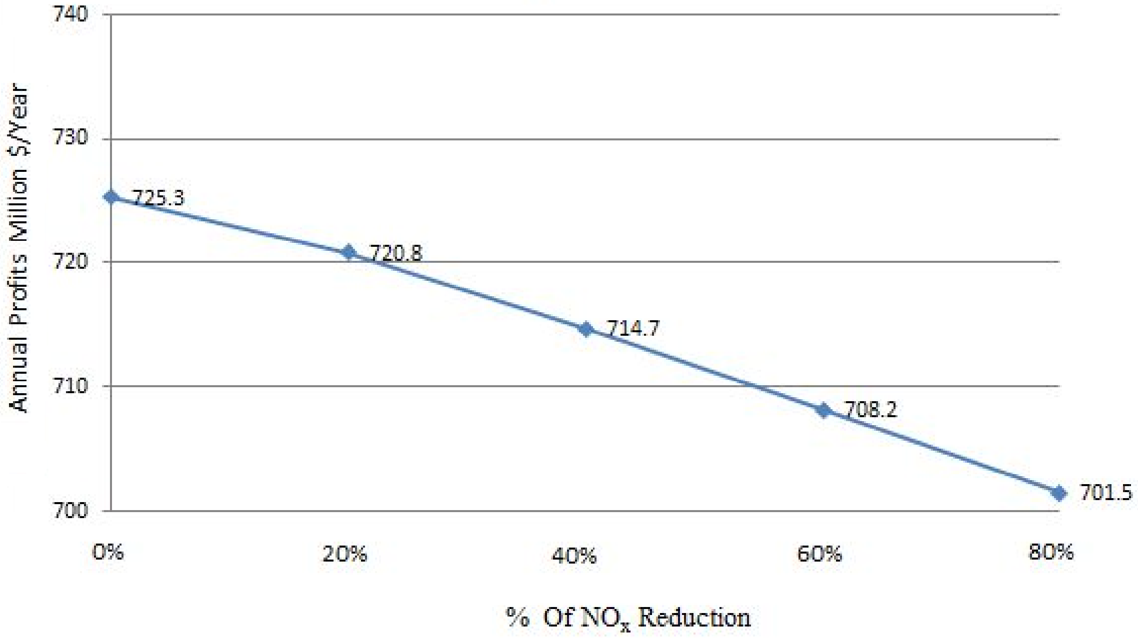


Figure 4.8: Effect of NO_X reduction percentage on profits

4.5 Sensitivity Analysis

In this study, sensitivity analysis of final product prices, products demand, switching cost and NO_X reduction technology cost were performed to analyze the impact on the profit for the different case studies shown in the previous section.

Case A:

For case A there is no NO_X reduction required. Meaning that our reduction target for Case A is 0% in NOx reduction. However, for this base case we will study the effect of inflation/deflation in the final product prices. The model tries to satisfy demand of each product by manipulating inlet flow rate for each unit to satisfy the demand. For an increase of 15% in final products price compared to the base case, the profit increases to about $1217 MM/yr while it decreases to about $233 millions/yr if the final products price decreases by 15%. The profits with original prices (0% increase in product prices) is $725 MM/yr. That means the profits increased by around 68% of original profits when the product prices increases by 15%. For the drop of 15% in product prices, the profits drop to $233 MM/yr which is a drop of 68% in profits compared to the normal case with the original prices. So we can see and predict how much our profits will change when the product prices changes.

Table 4.10: Inflation / Deflation effect of products prices

Profit (million $/yr)			
15% increase in selling price of products	**15% decrease in selling price of products**	**30% increase in selling price of products**	**30% decrease in selling price of products**
1217.4	233.1	1709.6	(-259)

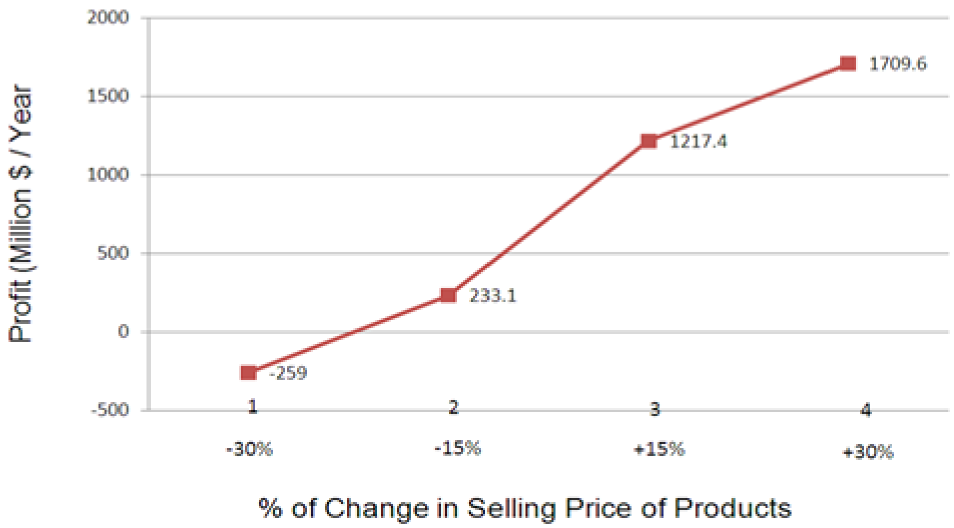


Figure 4.9: Inflation / Deflation effect of products prices

Looking at the 30% incrtaese or decrease in product prices, when the product prices increase by 30% we see that profits will increase to $1709 MM/yr that is equivalent to more than double the original profits by almost a factor of 1.4. However, we can see at 30% decrease in product prices, the refinery loses reaches $-259 MM/yr. This negative value indicates that the refinery is not making any profit. However, the refinery is losing 259 million dollar every year. It means there is a critical price for the products of the refinery where the refinery should not go below it and must have a safe margin above their critical prices to avoid loses.

Case B:

The effect of demand growth is studied and albeit the final products quantity is affected. Any increase in demand will lead to a change in flow rates which means that balancing is taking place in order to meet demand and a certain reduction target. The effect of final product selling price (increase by 15% and 30% in the price or decease by15% and 30%) is studied as in the previous case. In addition, effect of an increase by 15% and 30% or decrease by 15% and 30% in the switching costs to new fuel and SCR technology costs are investigated. SCR cost is considered as \$6,487/ton of NO_x removed as mentioned by Hatton and Bullions (2008). The mentioned cost is based on USA market, labor cost and it includes annual capital and operating cost. As noticed, any increase or decrease either on final product selling price or switching cost and SCR technology cost does not affect the number of units to be switched to run with new fuel or the amount of NO_X removed by SCR. The amount of each final product does not change much except when the demand change. The only affected variable is the profit as shown in the table 4.10, 4.11 & 4.12. The profit obviously increases with increasing price of final products and decreases with increasing the cost of switching to new fuel or increasing the cost of the SCR technology.

Table 4.11: Profit changes for the case with change in new fuel Cost

	Profit (million \$/yr)			
%NO_X Reduction	**30% decrease in new fuel Cost**	**15% decrease in new fuel Cost**	**15% increase in new fuel Cost**	**30% increase in new fuel Cost**
20 %	722.4	721.6	720	719.74
40 %	718.13	716.4	713.8	713.4
60 %	712.4	710.3	707.6	707.3
80%	702.2	701.0	700.7	700.13

Figure 4.10 and 4.11 show the sensitivity analysis results for price inflations. As seen earlier, it is clear that final product price has the major effect on the profit. However, for case B where the reduction target increases, we are assuming the product prices are fixed as per the original values but we assume changes in cost of switching and SCR technology. Looking at figure 4.10, it shows the variation in total profits for each reduction target as the cost of fuel switching increases or decreases. For example, for the 20% reduction, we noticed that for increase in fuel switching cost by 15%, the annual profits will drop to $720 MM. When the cost of switching increase to 30%, it shows that the profits will drop more to $719.74 MM/yr. This shows about a drop of $0.018 MM$/yr per 1.0% increase in fuel switching price. We can see that the drop in profits due to increase in cost of fuel switching is not very risky based on the values we got. We can see from figure 4.10 other reduction targets for the 40%, 60% and 80%. The slopes of the lines are very small indicating a low risk for price increase for the fuel switching cost.

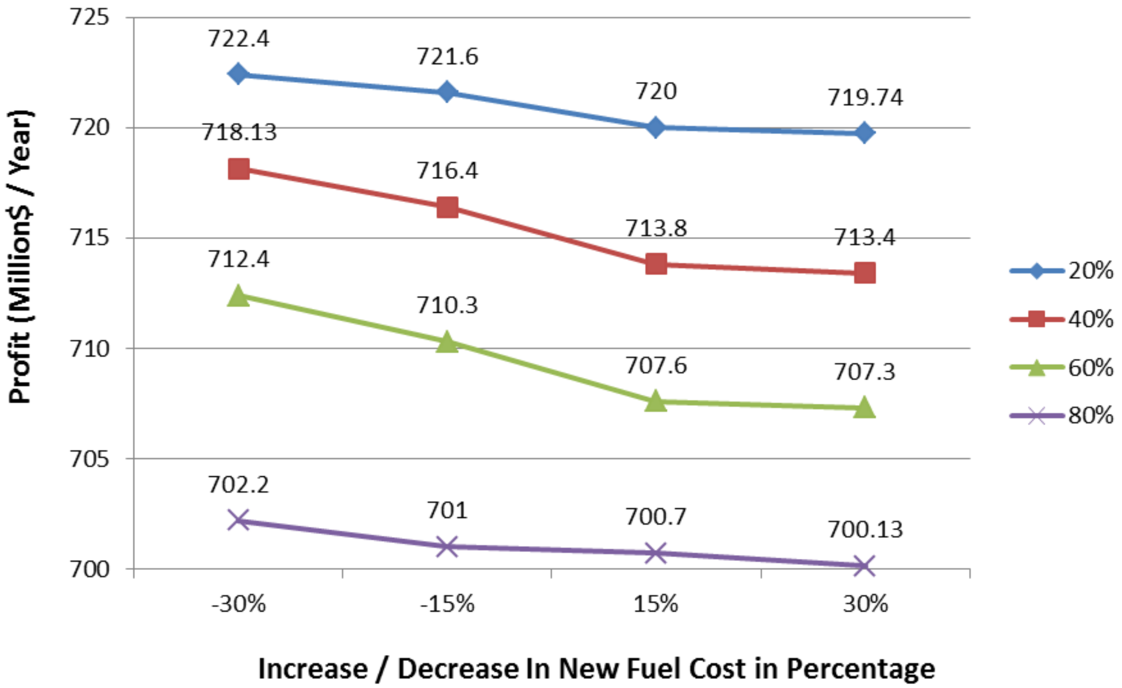


Figure 4.10: Profit changes results for changes in cost of new fuel

Table 4.12: Profit changes results for Case with change in SCR Cost

	Profit (million $/yr)			
%NO_X Reduction	**30% decrease in SCR Cost**	**15% decrease in SCR Cost**	**15% increase in SCR Cost**	**30% increase in SCR Cost**
20	720.8	720.8	720.8	720.8
40	714.7	714.7	714.7	714.7
60	712.7	710.3	707.6	707
80	708.2	704.7	698.5	695.4

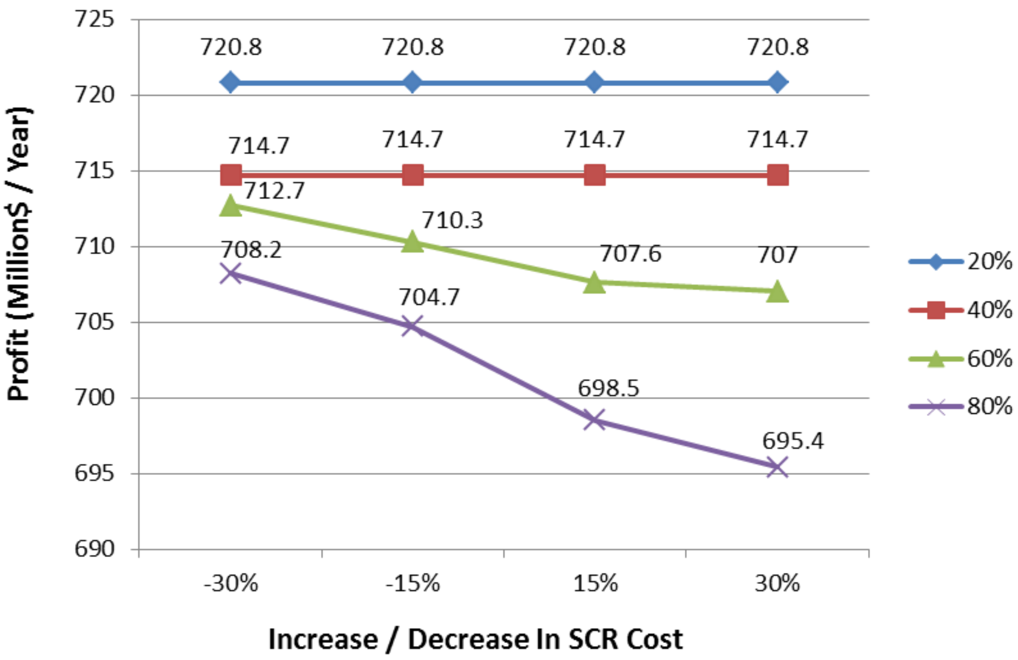
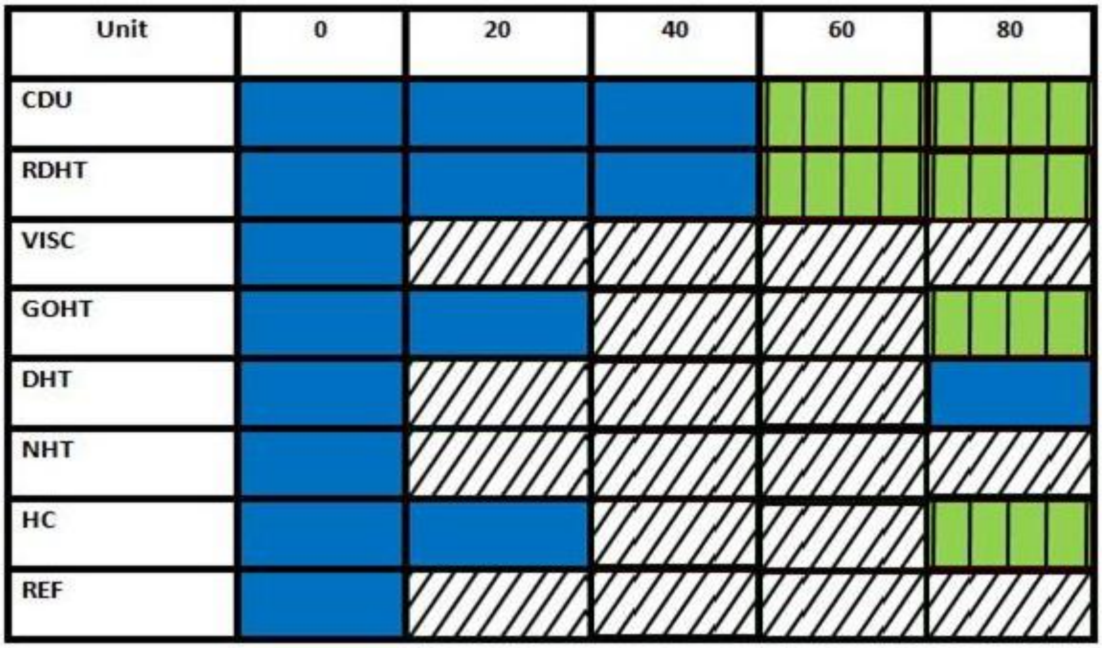


Figure 4.11: Shows the Sensitivity Results for SCR Technology Cost Changes (percentage wise)

It is clear from figure 4.11 that the effect of NO_X removal by SCR is more significant on the profit at higher reduction target. This is expected because more NO_X will be removed as more reduction is required. For the 20% reduction target, we see that the profits is the same for all increase/decrease percentages of the SCR technology cost and this is expected for the 20% reduction target. As we know already, at the 20% and 40% reduction targets, the model did not select the use of SCR technology for any of the eight units in the refinery. This leads to the conclusion that the profits for the cases of NO_X reduction by 20% and 40% are independent of the cost of the SCR technology since the model did not select them for use. However, for the 60% and 80%, the model selected some units to work with SCR technology in order to reach higher levels of NO_X reduction. We can see that the profits for the 60% and 80% are changing as we change the cost of the SCR technology. For example, for 80% reduction target, the model selected four units to work with the SCR technology. The profits at the 30% decrease in SCR technology cost is \$708.2 MM/yr while at the 30% increase of the SCR technology cost the profits drop to \$695.4 MM/yr. This gives us a very important conclusion. It shows that the profits will drop roughly by \$0.213 MM/yr for each 1.00% increase in the cost of the SCR technology. This can help the refinery to predict the business loses or gains as the SCR technology cost changes in the market. It can assist in estimating the risk involved in the use of other technologies and making a comparison among other technology to select the best one with lower risk in affecting the refinery profits. For the case of the 80% reduction target of NO_X, SCR was responsible for the removal of around 55% of the total NO_X produced by the refinery. Since the cost of the SCR is proportional to the total NO_X removed by this technology, we see for the 80% reduction target case, the profits are more sensitive to the increase/decrease in the SCR cost. However, for the 60% reduction target case, we see that the profits are less sensitive than the 80% reduction target case. This is because in the 60% reduction target, the SCR technology is responsible for the removal of around only 30% of the of the air pollutant (NO_X).



Unit	0	20	40	60	80
CDU	🟦	🟦	🟦	🟩	🟩
RDHT	🟦	🟦	🟦	🟩	🟩
VISC	🟦	▨	▨	▨	▨
GOHT	🟦	🟦	▨	▨	🟩
DHT	🟦	▨	▨	▨	🟦
NHT	🟦	▨	▨	▨	▨
HC	🟦	🟦	▨	▨	🟩
REF	🟦	▨	▨	▨	▨

Figure 4.12: Summary of Results

🟦 **Current fuel**

▨ **New fuel**

🟩 **Application SCR Technology**

Figure 4.12 gives a summary of all results for different reduction targets. The blue color represents that the unit is still using the old fuel which is fuel oil #6. The white box with black slopped lines represents switching to new fuel while the green color box with black straight lines represents application of NO_X reduction technology (SCR).

4.6 Summary

A general refinery planning model was developed to meet product demands with quality specifications and at the same time meet NO_X reduction targets. Different NO_X mitigation options were considered in order to look for different ways of minimizing cost and maximizing profits. It also gives the model more flexibility for finding different solutions of NO_X reduction. These methods are flow rate balancing, fuel switching and NO_X reduction technology. It was shown that, in order to reduce NO_X without fuel switching or NO_X SCR technology, the model tends to blend streams into the most profitable pool unless demand of some product needs to be met. This kind of flow rate balancing can achieve up to small reduction in NO_X emissions without considering quality constraints. When product specifications are taken into account, only very small reduction in NO_X is achieved by decreasing slightly the inlet flow rate for the unit that emits more NO_X.

For higher reduction targets up to 40%, fuel switching is the option of choice. The final products quantity and quality remain unchanged. The profit is affected by the cost changes of the new fuel. The study shows also that any increase or decrease for final product selling prices or retrofit cost affect the profit.

For NO_X reduction of more than 40%, the SCR technology is a promising option since it can achieve up to 90% reduction. The profit is negatively affected when using the

SCR method because it is more expensive than fuel switching. The effect of increase or decrease in the total cost of SCR including operating cost and maintenance cost can affect the final profits.

Up to 40% NO_X reduction can be achieved by switching as shown in the 20% and 40% NO_X reduction target cases. It is fevered for low NO_X reduction percentage to use fuel switching method instead of SCR Technology. The reason for that is the low cost of fuel switching compared to the use of SCR technology.

However, SCR application was selected at the next cases of 60% and 80% reduction targets. The use NO_X reduction technology is a better alternative to achieve high percentage of NO_X reduction. No NO_X reduction technology needs to be applied if the reduction target is 40% or less.

To sum up, the planning model tends to satisfy the product demand with quality specifications. Flow rate balancing is not a good option to reduce NO_X emission if quality constraints are added into the model. Fuel switching can achieve up to 40% NO_X reduction and beyond that, NO_X SCR technology processes should be applied.

Appendix A

Table A.1: Arab Light Crude Oil Data for Volume % Removed at Each Temperature and API Versus cut Temperature

Cut Temperature (F)	Volume %	Accum. Volume %	API	Mid. Volume
	2.2	1.1		2.2
200	7	5.7	78.8	9.2
315	11.3	14.85	59.5	20.5
400	9.1	25.05	49.5	29.6
500	11.6	35.4	42.1	41.2
600	10.1	46.25	35.4	51.3
700	9.5	56.05	28.6	60.8
800	5.9	63.75	25.4	66.7
900	8.7	71.05	21.5	75.4
1050	10.2	80.5	17.6	85.6
1200	14.4	92.8	5	100

Table A.2: Arab Light Crude Oil Data for Nitrogen & Sulfur Contents Versus cut Temperature

Cut Temperature (F)	Nitrogen Content ppm	Sulfur Content Wt.%
200	0.5	0.0184
340	0.5	0.0362
450	0.5	0.104
700	57.0	1.4000
800	500	2.321
900	909.0	2.50
1050	1406	2.80
1200	3340	4.17

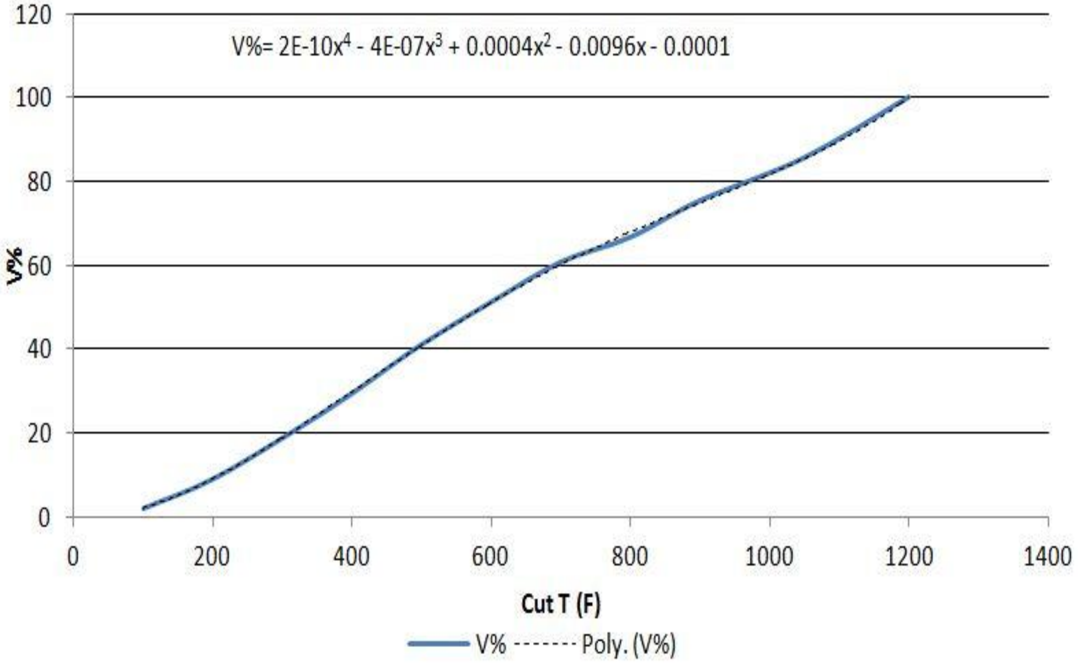


Figure A.1: Accumulative Volume % removed vs Cut Temperature for AL Crude Oil

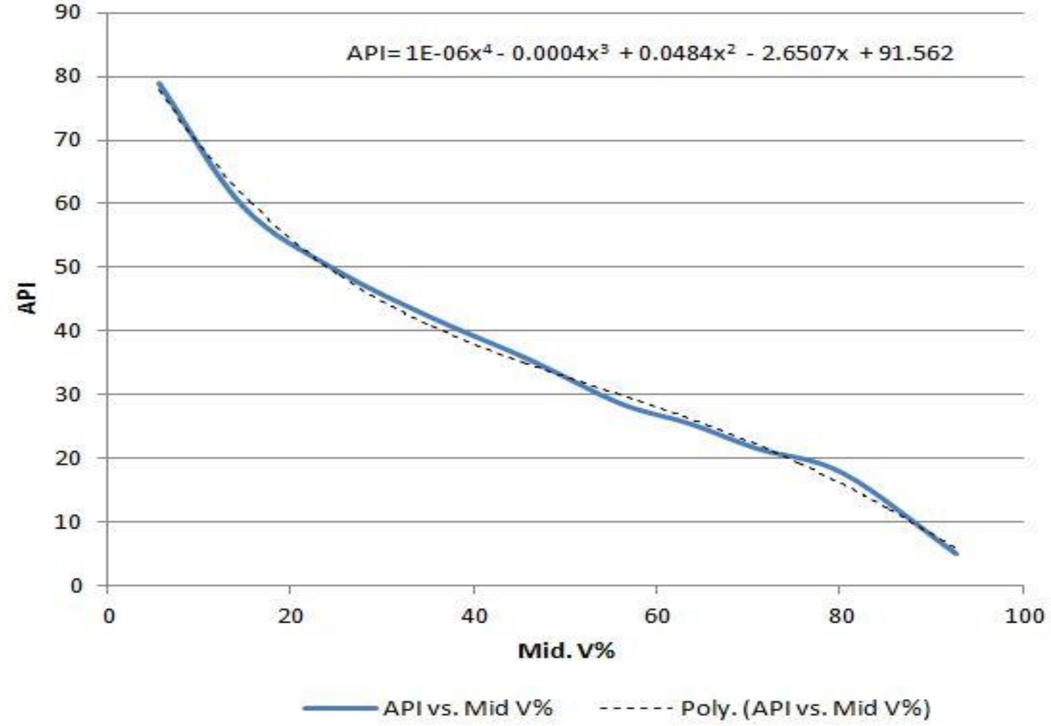


Figure A.2: API as a function of mid. V% for AL Crude Oil

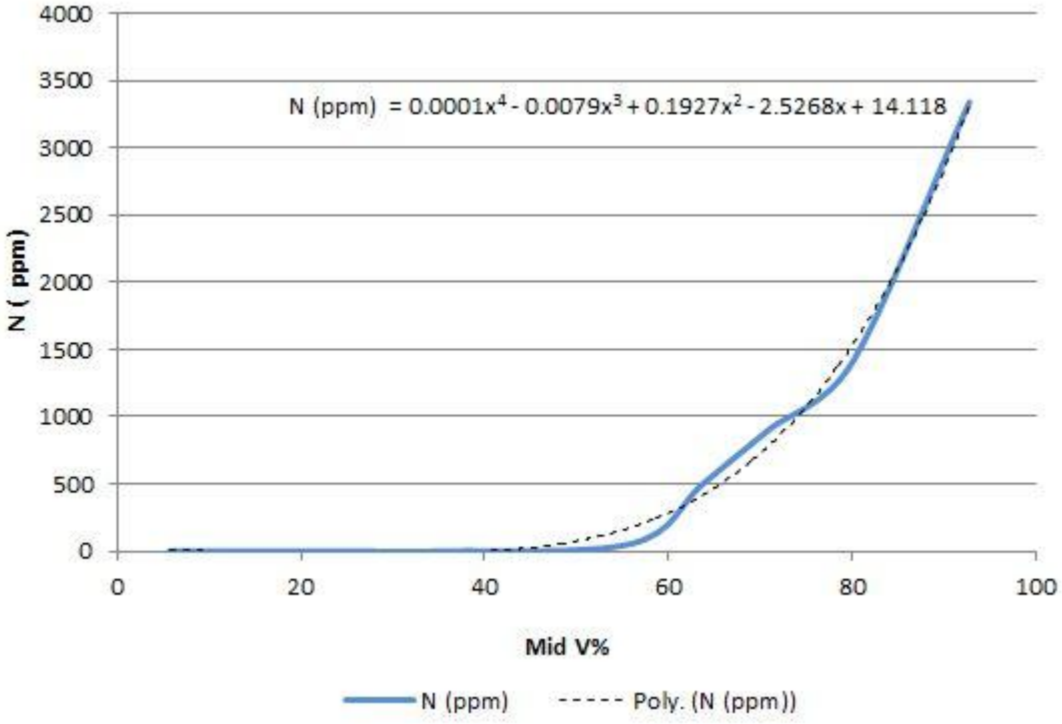


Figure A.3: N_2 Content Versus Cut Temperature for AL Crude Oil

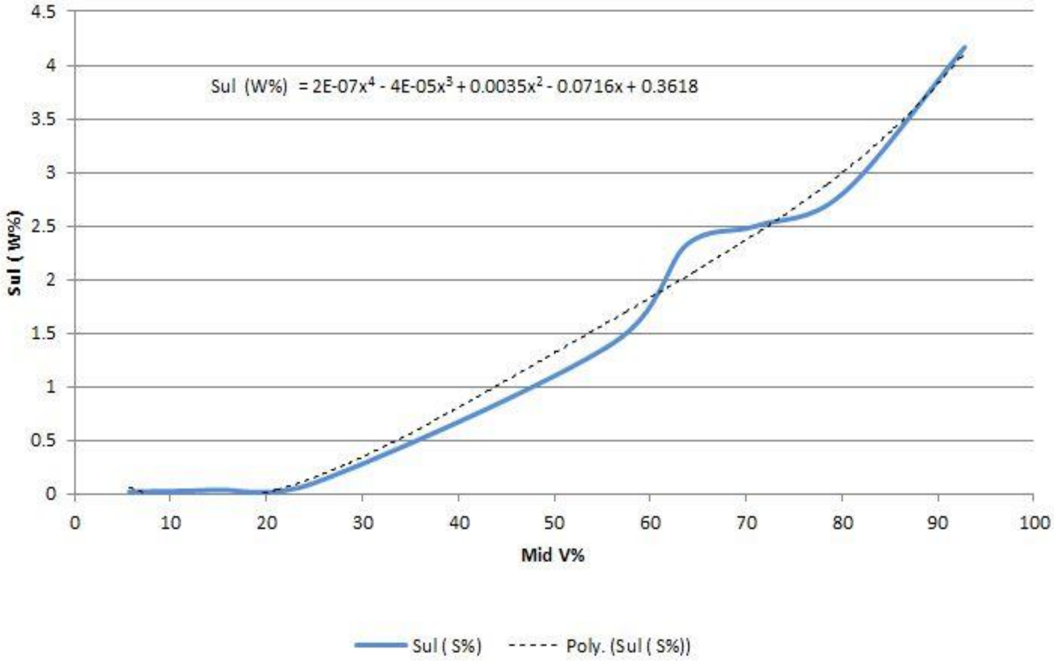


Figure A.4: Sulfur Content Wt% Versus Cut Temperature for AL crude

APPENDIX B

GAMS CODE

```
* Crude Distilation Unit CDU.mod


* his submodel is for calculating utilities etc. for crude units.

* Product yields and properties for a CDU are always calculated from assay

* Products: LSR, HSR, Kerosene,SRDiesel, LVGO, HVGO, VacResid

* Parameters: Cut1(180), Cut2(400), Cut3(530), Cut4(675), Cut5(900), Cut6(1050)


* Feed Crude Volume flowrate and end point cuts for products

Parameter RateV Rate in Volum BBl        /100000/

        LSREP  LSRN End Point (F)       / 180 /

        HSREP  HSRN End Point (F)       / 400 /

        KeroEP Kerosene End Point (F)   / 530 /

        SRDEP  SR Diesel End Point (F)  / 675 /

        LVGOEP LVGO End Point (F)       / 900 /

        HVGOEP HVGO End Point (F)       / 1050 /;

* Mid Volume %

Parameter Gas  /1.80/

        LSRV   ,LSRMV

        HSRV    ,HSRMV

        KeroV   ,KeroMV

        SRDV    ,SRDMV

        LVGOV   ,LVGOMV
```

```
        HVGOV   ,HVGOMV
        VRsdV   ,VRsdMV;

* Calculating Mid Volume % for all products from the EP's
* ProdV = 8.15312E-11*(EP^4) -2.84324E-07*(EP^3) +0.000324992*(EP^2)
*         -0.047271899*(EP)   + 4.040637061

LSRV  = 8.15312E-11*LSREP**4 -2.84324E-07*LSREP**3
LSRMV = (LSRV+Gas) / 2 ;
HSRV  = -2.84324E-07*HSREP**3  -0.047271899*HSREP
HSRMV = ( LSRV + HSRV ) / 2 ;
KeroV =  -2.84324E-07*KeroEP**-0.047271899*KeroEP
KeroMV= ( HSRV + KeroV ) / 2 ;
SRDV  = -2.84324E-07*SRDEP**3 -0.047271899*SRDEP
SRDMV = ( KeroV + SRDV ) / 2 ;
LVGOV = -2.84324E-07*LVGOEP**3  -0.047271899*LVGOEP;
LVGOMV= ( SRDV + LVGOV ) / 2 ;
HVGOV = -2.84324E-07*HVGOEP**3  -0.047271899*HVGOEP;
HVGOMV= ( LVGOV + HVGOV ) / 2 ;
VRsdV = 100 ;
VRsdMV= ( HVGOV + VRsdV ) / 2 ;

Display LSRMV,HSRMV,SRDMV,LVGOMV,HVGOMV,VRsdMV;
* API
Parameter LSRAPI,LSRSG
        HSRAPI ,HSRSG
```

```
      KeroAPI,KeroSG
      SRDAPI,SRDSG
      LVGOAPI,LVGOSG
      HVGOAPI,HVGOSG
      VRsdAPI,VRsdSG;
* Calculating API for all products from the Mid Vol%
* ProdAPI = 7.19024E-06*(EP^4) +0.108882599*(EP^2)
*        -3.564876491*(EP)
LSRAPI  = -0.0015436414*LSRMV**3  +0.113288448*LSRMV**2  -3.778147973*LSRMV;
LSRSG =141.5/(LSRAPI +131.5);
HSRAPI  = -0.0015436414*HSRMV**3  +0.113288448*HSRMV**2  -3.778147973*HSRMV;
HSRSG =141.5/(HSRAPI +131.5);
KeroAPI = -0.0015436414*KeroMV**3 +0.113288448*KeroMV**2 -3.778147973*KeroMV
KeroSG=141.5/(KeroAPI+131.5);
SRDAPI  = -0.0015436414*SRDMV**3  +0.113288448*SRDMV**2  -3.778147973*SRDMV;
SRDSG =141.5/(SRDAPI+131.5);
LVGOAPI = -0.0015436414*LVGOMV**3 +0.113288448*LVGOMV**2 -
3.778147973*LVGOMV;
LVGOSG=141.5/(LVGOAPI+131.5);
HVGOAPI = -0.0015436414*HVGOMV**3 +0.113288448*HVGOMV**2 -
3.778147973*HVGOMV;
HVGOSG=141.5/(HVGOAPI+131.5);
VRsdAPI = 7.19024E-06*VRsdMV**4 +0.113288448*VRsdMV**2 -3.778147973*VRsdMV;
VRsdSG=141.5/(VRsdAPI+131.5);
* Specific gravity (SG) for all products
```

```
* Sulfur content
Parameter LSRS
        HSRS
        KeroS
        SRDS
        LVGOS
        HVGOS
        VRsdS;
* Calculating Sulfur conten for all products from the Mid Vol%
* ProdS = 2.0301E-07*(MV^4) +0.001756678*(MV^2)
*         -0.01690124*(MV)
LSRS  = 2.0301E-07*(LSRMV**4) +0.001849373*(LSRMV**2)  -0.02036269*LSRMV;
HSRS  = 2.0301E-07*(HSRMV**4) +0.001849373*(HSRMV**2)  -0.02036269*HSRMV;
KeroS = 2.0301E-07*(KeroMV**4) +0.001849373*(KeroMV**2) -0.02036269*KeroMV;
SRDS  = 2.0301E-07*(SRDMV**4) +0.001849373*(SRDMV**2)  -0.02036269*SRDMV;
LVGOS = 2.0301E-07*(LVGOMV**4) -3.25656E-05*(LVGOMV**3)
+0.001849373*(LVGOMV**2) -0.02036269*LVGOMV +0.050579083;
HVGOS = 2.0301E-07*(HVGOMV**4) -3.25656E-05*(HVGOMV**3)
+0.001849373*(HVGOMV**2) -0.02036269*HVGOMV +0.050579083;
VRsdS = 2.0301E-07*(VRsdMV**4) +0.001849373*(VRsdMV**2) -0.02036269*VRsdMV;
* Nitrogen content
Parameter LSRN
        HSRN
```

```
        KeroN
        SRDN
        LVGON
        HVGON
        VRsdN;
* Calculating Nitrogen conten for all products from the Mid Vol%
* ProdN = 6.76957E-09*(EP^4) -2.16091E-05*(EP^2)
*        +0.000261549*(EP)
LSRN  = 6.76957E-09*LSRMV**4 -2.2968E-05*LSRMV**2  +0.000304355*LSRMV;
HSRN  = 6.76957E-09*HSRMV**4 -2.2968E-05*HSRMV**2  +0.000304355*HSRMV;
KeroN = 6.76957E-09*KeroMV**4 -2.2968E-05*KeroMV**2 +0.000304355*KeroMV;
SRDN  = 6.76957E-09*SRDMV**4 -2.2968E-05*SRDMV**2  +0.000304355*SRDMV;
LVGON = 6.76957E-09*LVGOMV**4 -2.2968E-05*LVGOMV**2 +0.000304355*LVGOMV;
HVGON = 6.76957E-09*HVGOMV**4 -2.2968E-05*HVGOMV**2 +0.000304355*HVGOMV
;
VRsdN = 6.76957E-09*VRsdMV**4 -2.2968E-05*VRsdMV**2 +0.000304355*VRsdMV;
*  Volume %
Parameter FLPG Vol folw rate of Off-Gas
        FLSRN  Vol folw rate of LSR Naph
        FHSRN  Vol folw rate of HSR Naph
        FKERO  Vol folw rate of Kero
        FDIESEL  Vol folw rate of SR Disel
        FLVGO  Vol folw rate of LVGO
        FHVGO  Vol folw rate of HVGO
        FRSD  Vol folw rate of VRsd;
FLPG   =Gas*RateV/100;
```

```
FLSRN  =(LSRV-Gas)*RateV/100;

FHSRN  =(HSRV-LSRV)*RateV/100;

FKero  =(KeroV-HSRV)*RateV/100;

FDiesel=(SRDV-KeroV)*RateV/100;

FLVGO  =(LVGOV-SRDV)*RateV/100;

FHVGO  =(HVGOV-LVGOV)*RateV/100;

FRSD  =(VRsdV-HVGOV)*RateV/100;

* Mass Flow Rates

Parameter RateWC3

          RateWiC4

          RateWnC4

          RATEWLSRN

          RATEWHSRN

          RATEWKERO

          RATEWDIESEL

          RATEWLVGO

          RATEWHVGO

          RATEWRESD;

* SG for C3, iC4 & nC4 are 0.5081, 0.5626 & 0.5835 respectivly.

RateWnC4 =(0.48*RateV/100)*0.5835*0.3502;

RATEWLSRN =FLSRN*LSRSG*.3502;

RATEWHSRN =FHSRN*HSRSG*.3502;

RATEWKERO=FKERO*KEROSG*.3502;

RATEWDIESEL =FDIESEL*SRDSG*.3502;

RATEWLVGO=FLVGO*LVGOSG*.3502;

RATEWHVGO=FHVGO *HVGOSG*.3502;
```

```
RATEWRESD=FRSD*VRSDSG*.3502;

* Products Properties

*______________________________________________________________________________
_

* L Naphtha

Parameter ARO2    /6.1/

        NAPH2   /17.7/

        OLE2    /0/

        RVP2    /7.95/

        RON2    /70.2/

        MON2    /55/

        V1502   /64.3/

        V2002   /100/

        V3002   /100/

        V4002   /100/

* H Naphtha

        RON3    /59.7/

        MON3    /55/

        V1503   /0/

        V2003   /15.4/

        V3003   /53.8/

        V4003   /92.3/

*Kero

        VABP4   /465/

        FLSH4   /180/

        NAPH4   /0.1/
```

```
          ARO4    /27.7/
          SMK4    /17.5/
          FRZ4    /-23/
          CS1224  /1.69/
          CS2104  /1.12/
          NI4     /0/
          VAN4    /0/
          CCR4    /0/
          OLE4    /0/
          V3004   /0/
          V4004   /11.8/
          V5004   /70.6/
          V6504   /100/
*Deisel
          VABP5   /604/
          FLSH5   /249/
          ARO5    /4.4/
          CS1225  /4.58/
          CS2105  /1.77/
          NI5     /0.00538/
          VAN5    /0.00663/
          CCR5    /0.00901/
          OLE5    /0/
          V3005   /0/
          V4005   /0/
          V5005   /0/
```

```
        V6505   /75.7/

*LVGO

        VABP6   /786/

        Flsh6   /305/

        NI6     /0.2/

        VAN6    /0.3/

        CCR6    /0.4/

        V6506   /0/

        OLE6    /0/

        Por6    /81/

        CS1226  /35.68/

        CS2106  /6.18/

*HVGO

        VABP7   /972/

        Flsh7   /337/

        NI7     /1.3/

        VAN7    /2.2/

        CCR7    /1.6/

        V6507   /0/

        OLE7    /0/

        Por7    /111/

        CS1227  /2077.9/

        CS2107  /60.27/

* Vac Residue

        VAN8     VANADIUM       /151.2/

        NI8      NICKEL         /61.1/
```

```
        CS1228   Viscosity @122F/4.19E+8/

        CS2108   Viscosity @210F/5111.3/

        POR8     Pour point     /130/

* Utility


PARAMETER EF/1.04/

         EF2/

         EF3/;


Parameter
PowerCDU,LPSCDU,CWCDU,FuelCDU,CapitalCDU,NOXCDU,NOXCDU2,NOXCDU3;

PowerCDU  = RateV;

LPSCDU    = RateV;

CWCDU     = RateV;

FuelCDU   = RateV;

CapitalCDU= -130*(RateV/100000)**0.65;

NOXCDU=EF*(-FuelCDU);

NOXCDU2=EF2*(-FuelCDU);

NOXCDU3=EF3*(-FuelCDU);

BINARY VARIABLE X1CDU,X2CDU,X3CDU;

VARIABLE TNOXCDU;

EQUATION Q11,QQ11,QQQ11;

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* RDHT.mod  -  Vacuum Residue Hydrotreater


* Use this submodel for hydrotreating with minimal cracking

* Products: Naphtha, Distillate, LSFO   $ Naph:375-F, Dist:375-650F, LSFO:+650F


* Feed (Residue from the CDU) properties

Parameter RateVRDHT Vol flowrate of feed from CDU Residue

        RateWRDHT   Mass flow rate from CDU Residue

        SGRDHT      Specific gravity of feed from CDU Residue

        APIRDHT     API of feed from CDU Residue

        SulRDHT     SULFUR CONTENT (%) of feed from CDU Residue

        NITRDHT     NITROGEN % of feed from CDU Residue

        VANRDHT     VANADIUM % of feed from CDU Residue

        NIRDHT      NICKEL of feed from CDU Residue

        FlshRDHT    Flash point of feed from CDU Residue

        VABPRDHT    Volume average boiling point of feed from CDU Residue

        C5IRDHT     C5 insoluble of feed from CDU Residue

        CCRRDHT     mass% of Conradson carbon of feed from CDU Residue;

RateVRDHT = FRSD;

SGRDHT    = VRsdSG;

APIRDHT   = VRsdAPI;

RateWRDHT = RateVRDHT*SGRDHT*.3502;

SulRDHT   = VRsdS;

NITRDHT   = VRsdN;
```

```
VANRDHT   = VAN8;

NIRDHT    = NI8;

CS122RDHT = CS1228;

CS210RDHT = CS2108;

PORRDHT   = POR8;

FlshRDHT  = Flsh8;

VABPRDHT  = VABP8;

C5IRDHT   = C5I8;

CCRRDHT   = CCR8;

* Products Yeild

Parameter SCFHYDRDHT

        WTFRHYDRDHT      H2 mass fraction

        C3SRDHT

        IC4RDHT

        NC4RDHT

        NAPH            Naphtha mass fraction

        RateW1RDHT      Naph mass  flow rate

        Dist            Mid Distillate mass fraction

        RateW2RDHT      Distt mass  flow rate

        RateW3RDHT      Residue mass  flow rate

        RATEV1RDHT

        RATEV2RDHT

        RATEV3RDHT;

SCFHYDRDHT
=(140*SGRDHT+0.39*(VANRDHT+NIRDHT)+91.5*NITRDHT)*(2.72*SGRDHT-1.61);

WTFRHYDRDHT=(1/658.29)*(SCFHYDRDHT/SGRDHT);
```

```
H2RDHT     =-WTFRHYDRDHT*RateWRDHT/100;

H2SRDHT    =0.85031*SulRDHT*RateWRDHT/100;

NAPH       =(0.12*SulRDHT+0.0063*(VANRDHT+NIRDHT))*(2.035*SGRDHT-0.95);

GASRDHT    =0.67*NAPH*RateWRDHT/100;

C3SRDHT    =0.27*GASRDHT;

IC4RDHT    =0.05*GASRDHT;

NC4RDHT    =0.23*GASRDHT;

RateW1RDHT =NAPH*RateWRDHT/100;

Dist       =3.56*NAPH-0.16*NAPH**2;

RateW2RDHT =Dist*RateWRDHT/100;

RateW3RDHT =RateWRDHT-H2RDHT-H2SRDHT-GasRDHT-RateW1RDHT-RateW2RDHT;

*  Products Properties

* NAPHTHA (375-F)

Parameter APINRDHT    /51.5/

          SGNRDHT

          VABPNRDHT    /267/

          RVPNRDHT     /1.3/

          RONNRDHT     /55/

          MONNRDHT     /50/

          V150NRDHT    /2/

          V200NRDHT    /11/

          V300NRDHT    /0/

          V400NRDHT    /0/;

SGNRDHT = 141.5/(APINRDHT +131.5);

* Distillate (375-650F)

Parameter APIDRDHT    /35.5/
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```
        SGDRDHT
        VABPDRDHT    /502/
        ANLDRDHT     /150/
        CETDRDHT
        FRZDRDHT     /-5/
        PorDRDHT     /-10/
* FLSHDRDHT IS DEFINED BY USER (210-250F)
        FLSHDRDHT    /225/
        CS122DRDHT   /2.5/
        CS210DRDHT   /1.4/;
SGDRDHT = 141.5/(APIDRDHT +131.5);
CETDRDHT= (ANLDRDHT-32)/1.8-15.5;
Parameter SulNRDHT  SULFUR CONTENT IN NAPH
        SulDRDHT   SULFUR CONTENT IN MIDDLE DISTILLATE
        SulLSFO   SULFUR OF RESID FUEL OIL
        NITNRDHT   NITROGEN CONTENT OF NAPH
        NITDRDHT   NITROGEN CONTENT OF MIDDLE DISTILLATE
        NITLSFO   NITROGEN CONTENT OF RESID FUEL OIL
        SGLSFO    SG OF RESID FUEL OIL
        PORLSFO   POUR POINT OF RESID FUEL OIL
        VGCF      FEED VISCOSITY-GRAVITY CONST
        VGCRsd    RESID VISCOSITY-GRAVITY CONST
        CS210LSFO VISCOSITY AT 210 OF RESID FUEL OIL
        CS122LSFO VISCOSITY AT 122 OF RESID FUEL OIL
        VANLSFO   VANADIUM % of RESID FUEL OIL
        NILSFO    NICKEL of RESID FUEL OIL
```

```
         VABPLSFO  Volume average boiling point of RESID FUEL OIL
         FlshLSFO  Flash point of RESID FUEL OIL
         C5ILSFO   C5 insoluble of RESID FUEL OIL
         CCRLSFO   mass% of Conradson carbon of RESID FUEL OIL;
*NAPHTHA (375-F)
NITDRDHT =0.16*NITRDHT;
* RESIDUE (LSFO:+650F)
SGLSFO  =SGRDHT-0.0195*SGRDHT*WTFRHYDRDHT+0.012*WTFRHYDRDHT;
SulLSFO =(0.2*SulRDHT*RateWRDHT-SulNRDHT*RateW1RDHT-
SulDRDHT*RateW2RDHT)/RateW3RDHT;
NITLSFO =(0.69*NITRDHT*RateWRDHT-NITNRDHT*RateW1RDHT-
NITDRDHT*RateW2RDHT)/RateW3RDHT;
PORLSFO =PORRDHT/(0.6+0.0028*SulRDHT*PORRDHT);
VGCF =(SGRDHT-0.1244*LOG10(4.664*CS210RDHT-31))/(0.9255-
0.0979*LOG10(4.664*CS210RDHT-31))-0.0839;
VGCRsd=VGCF+0.56*(SGLSFO-SGRDHT);
CS210LSFO=(31+10**((0.9255*VGCRsd-SGLSFO+0.0776)/(0.0979*VGCRsd-
0.1162)))/4.664;
CS122LSFO=.85*CS122RDHT;
NILSFO  =1600*NIRDHT/RateWRDHT;
VANLSFO =1600*VANRDHT/RateWRDHT;
VABPLSFO=VABPRDHT-25;
*Volumetric flow rates
Parameter FNRDHT RDHT Naph
         FDRDHT  RDHT Distt
         FLSFO   RDHT VRD;
FNRDHT = RATEW1RDHT/(SGNRDHT*0.3502);
```

```
FDRDHT = RATEW2RDHT/(SGDRDHT*0.3502);
FLSFO  = RATEW3RDHT/(SGLSFO*0.3502);
* FDRDHT WILL SPLIT TO THREE STREAMS FDRDHTD(Diesel Pool) & FDRDHTF(FOil)
Variable FDRDHTD,FDRDHTF;
Equation Splt1;
Splt1.. FDRDHT =E= FDRDHTD + FDRDHTF;
* UTILITIES
Parameter GasLHVRDHT,FuelRDHT,LPSRDHT,PowerRDHT,CWRDHT,ChemRDHT,CapitalRDHT,NOXRDHT,NOXRDHT2,NOXRDHT3;;
GasLHVRDHT = GasRDHT*21;
LPSRDHT    = -RateVRDHT*(.004+.0000167*SCFHYDRDHT);
PowerRDHT  = -RateVRDHT*(.769+.006154*SCFHYDRDHT);
CWRDHT     = -RateVRDHT*(.0315+.0000923*SCFHYDRDHT);
CapitalRDHT= -(8.65+5+.01423*SCFHYDRDHT+(NIRDHT+VANRDHT-5)*.04)*(RateVRDHT/10000)**0.65;
BINARY VARIABLE X1RDHT,X2RDHT,X3RDHT;
VARIABLE TNOXRDHT;
EQUATION Q12,QQ12,QQQ12;
Q12..  TNOXRDHT =E= X1RDHT*NOXRDHT+X2RDHT*NOXRDHT2;
QQ12..  X2RDHT+X3RDHT =l= 1;
QQQ12.. X1RDHT+X2RDHT =E= 1;


*------------------------------------------------------------------------------------------
*------------------------------------------------------------------------------------------
*-------------------------------------------------------------------------------------------
* Viscobreaker
```

```
Parameter ConvVis  /0.8/
        SULVis   /0.1/
        APIVis /35.0/
        API1Vis /70.0/
        API2Vis / 50.0/
        API3Vis /35.0/;

Parameter RateWVis,
        H2SVis, GasVis
        RateW1Vis, RateW2Vis
        RateW3Vis, RateW4Vis
        Sul1Vis, Sul2Vis
        Sul3Vis, Sul4Vis,
        API4Vis, SG1Vis,
        SG2Vis, SG3Vis,
        SG4Vis, RateV1Vis,
        RateV2Vis, RateV3Vis,
        RateV4Vis;




RateWVis = RATEW3RDHT;
GasVis = 0.003*ConvVis*RateWVis;
RateW1Vis = 0.003*ConvVis*RateWVis;
```

```
RateW2Vis = 0.007*ConvVis*RateWVis;

RateW4Vis = RateWVis-H2SVis-GasVis-RateW1Vis

API4Vis = APIVis - 3.0;

SG1Vis = 141.5/(API1Vis + 131.5);

SG2Vis = 141.5/(API2Vis + 131.5);

SG3Vis = 141.5/(API3Vis + 131.5);

SG4Vis = 141.5/(API4Vis + 131.5);

RateV1Vis = RateW1Vis/(SG1Vis*0.3502);

RateV2Vis = RateW2Vis/(SG2Vis*0.3502);

RateV3Vis

Sul1Vis = SULVis;

Sul2Vis = SULVis;

Sul3Vis = SULVis;

Sul4Vis = SULVis;


*UTILITIES Viscobreaker

*______________________________________________________________________________

*______________________________________________________________________________

PARAMETERS

SGVis

RATEVVis

GASLHVVis

FUELVis

POWERVis

CWVis

HPSVis
```

```
BFWVis

CAPITALVis

NOXVis

NOXVis2

NoxVis3;


SGVis=141.5/(APIVis+131.5);

RATEVVis=RATEWVis/(SGVis*0.3502);

GasLHVVis=GasVis*21;

FuelVis = -RateVVis*0.088;

PowerVis = -RateVVis*0.47;

CWVis = -RateVVis*0.27;

HPSVis=+RateVVis*0.052;

BFWVis=-HPSVis;

CapitalVis = -30*(RateVVis/30000)**0.65;


NOXVis=EF*(-FuelVis);

NOXVis2=EF2*(-FuelVis);

NOXVis3=EF3*(-FuelVis);

BINARY VARIABLE X1Vis,X2Vis,X3Vis;



display H2SVis, RateWVis, FLSFO,GasVis, RateW1Vis, RateW2Vis,RateW3Vis,RateW4Vis,

        RateV1Vis, RateV2Vis, RateV3Vis, RateV4Vis;

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* GOHDS.mod  -  Gas Oil Hydrotreater


* Use this submodel for hydrotreating with minimal cracking
* Products: Naphtha, Distillate, HTGasOil
* Parameters: Severity(50)
* Severity 0=low pressure, high LHSV, 100=high pressure, low LHSV


*Feed Rate and Properties
Parameter
RateWGOHT,RateVGOHT,SGGOHT,APIGOHT,VABPGOHT,SULGOHT,NITGOHT,NIGOHT,VANGOHT
        CCRGOHT,FlshGOHT,V650GOHT,OLEGOHT,PorGOHT,CS122GOHT,CS210GOHT;
RATEVGOHT= FLVGO + FHVGO;
SGGOHT   = (FLVGO*HVGOSG+FHVGO*LVGOSG)/RATEVGOHT;
RATEWGOHT= RATEVGOHT*SGGOHT*.3502;
APIGOHT  = 141.5/SGGOHT-131.5;
VABPGOHT = (VABP6*FLVGO+VABP7*FHVGO)/RATEVGOHT;
SULGOHT  = (LVGOS*RATEWLVGO+HVGOS*RATEWHVGO)/RATEWGOHT;
NITGOHT  = (LVGON*RATEWLVGO+HVGON*RATEWHVGO)/RATEWGOHT;
NIGOHT   = (NI6*RATEWLVGO+NI7*RATEWHVGO)/RATEWGOHT;
VANGOHT  = (VAN6*RATEWLVGO+VAN7*RATEWHVGO)/RATEWGOHT;
CCRGOHT  = (CCR6*RATEWLVGO+CCR7*RATEWHVGO)/RATEWGOHT;
FlshGOHT = (Flsh6*FLVGO+Flsh7*FHVGO)/RATEVGOHT;
```

```
V650GOHT = (V6506*FLVGO+V6507*FHVGO)/RATEVGOHT;
OLEGOHT  = (OLE6*FLVGO+OLE7*FHVGO)/RATEVGOHT;
PorGOHT  = (Por6*FLVGO+Por7*FHVGO)/RATEVGOHT;
CS122GOHT= (CS1226*RATEWLVGO+CS1227*RATEWHVGO)/RATEWGOHT;
CS210GOHT= (CS2106*RATEWLVGO+CS2107*RATEWHVGO)/RATEWGOHT;

* YIELDS
Parameter SeverityGOHT/50/

KGOHT,convGOHT,SCFHYDGOHT,wtfrhydGOHT,H2GOHT,H2SGOHT,GasGOHT,C3SGOHT,IC4GOHT
        NC4GOHT,RateW1GOHT,APITGO,SGTGO,RateW3GOHT,RateW2GOHT;
KGOHT      =(VABPGOHT+460)**.3333/SGGOHT;
convGOHT   =4.5*SULGOHT;
SCFHYDGOHT =(290+20*convGOHT*(1-V650GOHT/100))*(1+.01*SeverityGOHT)+15*OLEGOHT+(VABPGOHT-700)*0.5;
wtfrhydGOHT= SCFHYDGOHT/65800/SGGOHT;
H2GOHT     =-wtfrhydGOHT*RateWGOHT;
H2SGOHT    =0.010625*SULGOHT*RateWGOHT*(1-(1-convGOHT/100)*(.2-.0016*SeverityGOHT));
GasGOHT    =(.004+.00001*convGOHT*convGOHT)*RateWGOHT;
C3SGOHT    =0.49*GasGOHT;
IC4GOHT    =(.001+.00015*convGOHT)*RateWGOHT;
NC4GOHT    =IC4GOHT*.7;
RateW1GOHT =(.02+.001*convGOHT)*RateWGOHT;
APITGO     =APIGOHT+.004*SCFHYDGOHT;
RateW2GOHT = RateWGOHT-H2GOHT-H2SGOHT-GasGOHT-IC4GOHT-NC4GOHT-RateW1GOHT-RateW3GOHT;
```

```
* PROPERTIES

* 400F & lighter naphtha
Parameter APINGOHT   /55/
          SGNGOHT
          RVPNGOHT    /4/
          RONNGOHT    /65/
          MONNGOHT    /60/
          NaphNGOHT   /18/
          OLENGOHT    /0/
          AroNGOHT    /12/
          V150NGOHT   /0/
          V200NGOHT   /35/
          V300NGOHT   /70/
          V400NGOHT   /100/
          VABPNGOHT   /0/
          SULNGOHT    /0/
          VANNGOHT    /0/
          CCRNGOHT    /0/ ;
SGNGOHT = 141.5/(APINGOHT +131.5);

* 400-650 Distillate
Parameter APIDGOHT    /36/
          SGDGOHT
          SULDGOHT    /.01/
```

```
      FlshDGOHT   /255/
      AroDGOHT    /10/
      PorDGOHT    /-10/
      CS122DGOHT  /5.3/
      CS210DGOHT  /2.0/
      V400DGOHT   /10/
      V500DGOHT   /48/
      V650DGOHT   /90/
      VABPDGOHT   /0/
      VANDGOHT    /0/
      CCRDGOHT    /0/
      CetDGOHT  ;
      SGDGOHT = 141.5/(APIDGOHT +131.5);
      CetDGOHT=1.85*APIDGOHT-14;


* 650+ gasoil
Parameter
VABPTGO,SULTGO,PorTGO,CS122TGO,CS210TGO,CCRTGO,NITTGO,OLETGO/0/,NITG
O/0/,VANTGO/0/;
VABPTGO = (SGTGO*(KGOHT+SeverityGOHT/100))**3-460;
CS210TGO= CS210GOHT;
CCRTGO  = CCRGOHT*(.6-.005*SeverityGOHT);
NITTGO  = NITGOHT*(.7-.005*SeverityGOHT);


*Volumetric flow rates
Parameter FNGOHT  GOHT Naph
```

```
          FDGOHT  GOHT Distt

          FTGO  GOHT VGO;

FNGOHT = RATEW1GOHT/(SGNGOHT*0.3502);

FDGOHT = RATEW2GOHT/(SGDGOHT*0.3502);

FTGO   = RATEW3GOHT/(SGTGO*0.3502);


* FDGOHT WILL SPLIT TO TWO STREAMS FDGOHTD (Diesel Pool) FDGOHTF (FOil Pool)

* FTGO WILL SPLIT TO TWO STREAMS FTGOFCC (FCC) FTGOHC (HC)

Positive Variable FDGOHTD, FDGOHTF,FTGOFCC,FTGOHC;

Equation Splt2,Splt3;

Splt2..  FDGOHT =E= FDGOHTD + FDGOHTF;

Splt3..  FTGO   =E= FTGOFCC + FTGOHC;

* UTILITIES

Parameter GasLHVGOHT,PowerGOHT,LPSGOHT,CWGOHT,FuelGOHT,ChemGOHT,CapitalGOHT,NOXGOHT,NOXGOHT2,NOXGOHT3;;

GasLHVGOHT = GasGOHT*21;

FuelGOHT   = -RateVGOHT*(.0846+.0000769*SCFHYDGOHT);

ChemGOHT   = -

RateVGOHT*(.0169+.00001539*SCFHYDGOHT+(NIGOHT+VANGOHT)*.0008);

CapitalGOHT= -(8.65+5+.01423*SCFHYDGOHT+(NIGOHT+VANGOHT-5)*.04)*(RateVGOHT/10000)**0.65;

NOXGOHT=EF*(-FuelGOHT);

NOXGOHT2=EF2*(-FuelGOHT);

NOXGOHT3=EF3*(-FuelGOHT);

BINARY VARIABLE X1GOHT,X2GOHT,X3GOHT;
```

```
VARIABLE TNOXGOHT;

EQUATION Q13,QQ13,QQQ13;

Q13..  TNOXGOHT =E= X1GOHT*NOXGOHT+X2GOHT*NOXGOHT2;

QQ13..  X2GOHT+X3GOHT =L= 1;

QQQ13.. X1GOHT+X2GOHT =E= 1;

*----------------------------------------------------------------------

*----------------------------------------------------------------------

* DHT_3Prod.mod;  Diesel/Kero Hydrotreater


*Products: DHTNaph,DHTKero, DHTDist     $ Naphtha:400-F, Kero:400-530F, Diesel:530-650F

*Parameters: Severity(20)

*Note that severity of 10-simple desulfurize, 90-aromatics saturation


*Feed Rate and Properties

Parameter
RATEVDHT,RATEWDHT,SGDHT,APIDHT,SULDHT,NITDHT,OLEDHT,ARODHT,V300DHT

         V400DHT,V500DHT,V650DHT;

NITDHT  = SRDN;

OLEDHT  = OLE5;

ARODHT  = ARO5;

V300DHT = V3005;

V400DHT = V4005;

V500DHT = V5005;

V650DHT = V6505;

* YIELDS
```

```
Parameter SEVERITYDHT/20/
Parameter
SCFHYDDHT,WTFRHYDDHT,H2DHT,H2SDHT,GASDHT,C3SDHT,IC4DHT,NC4DHT
      RATEW1DHT,DISTTWDHT,FRACKERODHT,RATEW2DHT,RATEW3DHT;
SCFHydDHT
=(150+OLEDHT*10+0.9*SULDHT*60)+(100+0.1*SULDHT*60+ARODHT*20)*SeverityDHT
/100;
WtFrHydDHT = SCFHydDHT/65800/SGDHT;
H2DHT      = -WtFrHydDHT*RateWDHT;
H2SDHT     = 0.010625*SULDHT*(0.95+SeverityDHT*0.0005)*RateWDHT;
GasDHT     = (0.005+0.000005*SeverityDHT*SeverityDHT)*RateWDHT;
C3SDHT     = 0.35*GasDHT;
IC4DHT     = 0.15*GasDHT;
NC4DHT     = 0.20*GasDHT;
RateW1DHT  = (0.001+0.0004*SeverityDHT)*RateWDHT;
DisttWDHT  = RateWDHT-H2DHT-H2SDHT-GasDHT-RateW1DHT;
* Products properties
* Naphtha:400-F
Parameter APINDHT/55/
      SGNDHT
      RVPNDHT /2/
      RONNDHT /65/
      MONNDHT /60/
      NAPHNDHT/18/
      ARONDHT /12/
      V150NDHT/0/
      V200NDHT/40/
```

```
        V300NDHT/70/
        V400NDHT/100/;
SGNDHT = 141.5/(APINDHT +131.5);

*  KERO 400-530 F
Parameter PORKDHT  /-40/
        FRZKDHT   /-30/
        FLSHKDHT  /180/
        CS122KDHT /1.3/
        CS210KDHT /0.75/
        V650KDHT  /100/
Parameter APIDISTT9 KERO + DSL API , APIKDHT ASSUME KERO API IS 9 MORE THAN DSL

SGKDHT,SULDISTT9,SULKDHT,ARODISTT9,AROKDHT,SMKKDHT,CETKDHT,V300KDHT,V400KDHT,V500KDHT;
APIDistt9  = APIDHT+.005*SCFHydDHT+.04*SeverityDHT;
APIKDHT      = APIDistt9+9*(1-FracKeroDHT);
SGKDHT       = 141.5/(APIKDHT+131.5);
SulDistt9  = SulDHT*(0.1-.0009*SeverityDHT);
SULKDHT      = SulDistt9/(FracKeroDHT+ 1.8*(1-FracKeroDHT));
AroDistt9  = AroDHT*(1-0.008*SeverityDHT);
AROKDHT      = AroDistt9/(FracKeroDHT+ 1.4*(1-FracKeroDHT));
SMKKDHT      = 0.8*APIKDHT-11;
CETKDHT      = 1.64*APIKDHT-15.4;

*  Diesel:530-650F
```

```
Parameter
GASLHVDHT,FUELDHT,LPSDHT,POWERDHT,CWDHT,CHEMDHT,CAPITALDHT,NOXDHT,NOXDHT2,NOXDHT3;

GASLHVDHT  = GasDHT*21;

FUELDHT    = -RateVDHT*(.0846+.0000769*SCFHydDHT);

LPSDHT     = -RateVDHT*(.004+.0000167*SCFHydDHT);

POWERDHT   = -RateVDHT*(.769+.006154*SCFHydDHT);

CWDHT      = -RateVDHT*(.0315+.0000923*SCFHydDHT);

CHEMDHT    = -RateVDHT*(.0169+.00001539*SCFHydDHT);

CAPITALDHT = -(8.65+.01423*SCFHydDHT)*(RateVDHT/10000+.0001)**0.65;

NOXDHT=EF*(-FUELDHT);

NOXDHT2=EF2*(-FUELDHT);

NOXDHT3=EF3*(-FUELDHT);

BINARY VARIABLE X1DHT,X2DHT,X3DHT;

VARIABLE TNOXDHT;

EQUATION Q14,QQ14,QQQ14;

Q14..  TNOXDHT =E= X1DHT*NOXDHT+X2DHT*NOXDHT2;

QQ14.. X2DHT+X3DHT =L= 1;

QQQ14.. X1DHT+X2DHT =E= 1;

*---------------------------------------------------------------------

*---------------------------------------------------------------------

*NHT_2PRD

*Two products;Lt naphtha and Hvy naphtha

*Parameter:LNEP(180)    usable range 150-200F


* Feed Rate and Properties
```

```
Parameter
RATEVNHT,SGNHT,RATEWNHT,SULNHT,OLENHT,ARONHT,NAPHNHT,RONNHT
        V150NHT,V200NHT,V300NHT,V400NHT;
RATEVNHT = FHSRN;
SGNHT    = HSRSG;
RATEWNHT = RATEVNHT*SGNHT*0.3502;
SULNHT   = HSRS;
ARONHT   = ARO3;
NAPHNHT  = NAPH3;
RONNHT   = RON3;
V150NHT  = V1503;
V200NHT  = V2003;
V300NHT  = V3003;
V400NHT  = V4003;
OLENHT   = OLE3;

* YIELDS
Parameter LNEPNHT/180/,SCFHYDNHT,WTFRHYDNHT,H2NHT,H2SNHT,GASNHT,
        RATENAPNHT,FRACLNNHT,RATEW1NHT,RATEW2NHT,RATEVNHT;
SCFHydNHT =125+8.3*OLENHT;
GasNHT    =0.003*RateWNHT;
RateNapNHT= RateWNHT-H2NHT-H2SNHT-GasNHT;
FracLNNHT =(V150NHT +(V200NHT-V150NHT)*(LNEPNHT-150)/50)/100;
RateW1NHT =RateNapNHT*FracLNNHT*0.88;
RateW2NHT =RateNapNHT-RateW1NHT;
```

```
* Products properties
* Lt Naphtha
Parameter RVPTLN/8/
        RONTLN/65/
        MONTLN/60/
        V200TLN/100/
        V300TLN/100/
        V400TLN/100/
        SGTLN;
SGTLN   = 0.67 +(LNEPNHT-150)*.0006;
Parameter AROTLN,NAPHTLN,V150TLN;
AROTLN  = ARONHT*(LNEPNHT-150)*.005;
NAPHTLN = (NAPHNHT+0.1*OLENHT)*(LNEPNHT-150)*.005;
V150TLN = V150NHT/FracLNNHT;

* Hvy Naphtha
Parameter V150THN/0/
         RVPTHN /4/
*Variable
Parameter
SGTHN,AROTHN,NAPHTHN,RONTHN,MONTHN,V200THN,V300THN,V400THN;
SGTHN  = (SGNHT-SGTLN*FracLNNHT)/(1-FracLNNHT);
AROTHN = ARONHT+0.1*OLENHT;
NAPHTHN= NAPHNHT+0.1*OLENHT;
RONTHN = RONNHT;
MONTHN = RONTHN-5;
```

```
V200THN= 100 -(100-V200NHT)/(1-FracLNNHT);
V300THN= 100 -(100-V300NHT)/(1-FracLNNHT);
V400THN= 100 -(100-V400NHT)/(1-FracLNNHT);


* Volumetric Flowrate of products
Parameter FTLN, FTHN;
FTLN  = RATEW1NHT/(SGTLN*0.3502);
FTHN  = RATEW2NHT/(SGThN*0.3502) + RateV2Vis;
* UTILITIES
Parameter
GASLHVNHT,FUELNHT,LPSNHT,POWERNHT,CWNHT,CHEMNHT,CAPITALNHT,NOXNHT,NOXNHT2,NOXNHT3;
GASLHVNHT = GasNHT*21;
FUELNHT   = -RateVNHT*(.0846+.0000769*SCFHydNHT);
NOXNHT   = -FUELNHT*(55/1000)*(1/0.02380952);
LPSNHT    = -RateVNHT*(.004+.0000167*SCFHydNHT);
POWERNHT  = -RateVNHT*(.769+.006154*SCFHydNHT);
CWNHT     = -RateVNHT*(.0315+.0000923*SCFHydNHT);
CHEMNHT   = -RateVNHT*(.0169+.00001539*SCFHydNHT);
CAPITALNHT= -(8.65+.01423*SCFHydNHT)*(RateVNHT/10000)**0.65;
NOXNHT=EF*(-FUELNHT);
NOXNHT2=EF2*(-FUELNHT);
NOXNHT3=EF3*(-FUELNHT);
BINARY VARIABLE X1NHT,X2NHT,X3NHT;
VARIABLE TNOXNHT;
EQUATION Q15,QQ15,QQQ15;
```

```
Q15..  TNOXNHT =E= X1NHT*NOXNHT+X2NHT*NOXNHT2;
QQ15..  X2NHT+X3NHT =L= 1;
QQQ15.. X1NHT+X2NHT =E= 1;
*------------------------------------------------------------------------------
*----------------------------------------------------------------------
* HydCrk.mod   -  Gas Oil Hydrocracker
* Full conversion hydrocracker-Jet Mode or diesel mode selected by user input

* Products: HCLtNaph, HCHvyNaph, HCKero,HCDiesel
* Parameters: Mode(1)
* MODE to be 1 for Diesel, 2 for Kero or in between
* Note : (1)Light Naphtha ~180F EP (2) Heavy Naphtha ~400F EP
*       (3)Kero/Jet ~530F EP      (4)Diesel ~650F EP
* Feed Properties:   VABP, OLE, NI, VAN

* Feed Rate and Properties
Parameter SGHC,APIHC,VABPHC,OLEHC,SULHC,NIHC,VANHC,CCRHC;
SGHC   = SGTGO;
APIHC  = 141.5/SGHC-131.5;
VABPHC = VABPTGO;
OLEHC  = OLETGO;
SULHC  = SULTGO;
NIHC   = NITGO;
VANHC  = VANTGO;
CCRHC  = CCRTGO;
Variable RateWHC,RateVHC;
```

```
Equation RateWHC1,RateVHC1;
RATEVHC1.. RATEVHC=E= FTGOHC;
RATEWHC1.. RATEWHC=E= RATEVHC*SGHC*0.3502;

*  YIELDS
Parameter
CONVHC/75/,ModeHC/1/,SCFHYDHC,WtFrHYDHC,LNapHC,HNHC,JetHC,DslHC,SubTotLQHC;
Variable H2HC,H2SHC,GasHC,C3SHC,IC4HC,NC4HC,SubTotLEHC,TotalHC,AdjFactHC
        RateWLNHC Light Naph,RateWHNHC Hvy Naph,RateWKEROHC Jet,RateWDIESELHC
Disel;
Equation H2HC1,H2SHC1,GasHC1,C3SHC1,IC4HC1,NC4HC1,SubTotLEHC1,TotalHC1
        AdjFactHC1,RateWLNHC1,RateWHNHC1,RateWKEROHC1,RateWDIESELHC1;

H2SHC1..      H2SHC    =E= 0.010625*(SULHC-0.0281+.0102*ModeHC)*RateWHC;
GasHC1..      GasHC    =E= (.001+.007*ModeHC)*RateWHC;
C3SHC1..      C3SHC    =E=  (.005+.002*ModeHC)*RateWHC;
IC4HC1..      IC4HC    =E=(.00682+.00347*ModeHC)*RateWHC;
NC4HC1..      NC4HC    =E=IC4HC*.818;
SubTotLEHC1..
SubTotLEHC=E=(H2HC+H2SHC+GasHC+C3SHC+IC4HC+NC4HC)/(RateWHC+.00001);

*  Unnormalized LN, HN etc below
LNapHC    = 1.86+3.39*ModeHC;
HNHC      = 0.26+5.77*ModeHC;
JetHC     = 6.91+34.86*ModeHC;
DslHC     = 91.16-45.58*ModeHC;
```

```
SubTotLQHC=(LNapHC+HNHC+JetHC+DslHC)/100;
TotalHC1..   TotalHC =E=SubTotLEHC+SubTotLQHC;
AdjFactHC1.. AdjFactHC=E=RateWHC/100*(SubTotLQHC-TotalHC+1)/SubTotLQHC;
RateWLNHC1..  RateWLNHC=E=LNapHC*AdjFactHC;
RateWHNHC1..  RateWHNHC=E=HNHC*AdjFactHC;
RateWKEROHC1.. RateWKEROHC=E=JetHC*AdjFactHC;
RateWDIESELHC1.. RateWDIESELHC=E=DslHC*AdjFactHC;

*  PROPERTIES
* Light Naphtha
Parameter RVPLNHC/10/,RONLNHC/82/,MONLNHC/77/,V150LNHC/70/,V200LNHC/80/
        V300LNHC/100/,V400LNHC/100/,KHC,KLNapHC,KHNHC,KJetHC,KDslHC,SGLNHC;
KHNHC  =KLNapHC-.75;
KJetHC =11.8+.4*(KHC-11.5);
KDslHC =KJetHC;
SGLNHC =(135+460)**.3333/KLNapHC;

* Heavy Naphtha
Parameter RVPHNHC/3/,RONHNHC/70/,MONHNHC/65/,V150HNHC/0/,V200HNHC/10/,
        V300HNHC/60/,V400HNHC/95/,SGHNHC,NAPHHNHC,AROHNHC;
SGHNHC  = (290+460)**.3333/KHNHC;
NAPHHNHC= 40+3*(11.6-KHNHC);
AROHNHC = 5+3*(11.6-KHNHC);

* Kero/Jet
* AROKEROHC IS DEFINED BY THE USER TO BE 18
```

```
Parameter SULKEROHC/.01/,FLSHKEROHC/165/,PORKEROHC/-70/,CETKEROHC/60/
        FRZKEROHC/-
65/,CS122KEROHC/1.5/,AROKEROHC/18/,SGKEROHC,SMKKEROHC;
SGKEROHC = (465+460)**.3333/KJetHC;
SMKKEROHC= 28+4*(KJetHC-11.4);

* Diesel
* CS210DIESELHC/1.2/ IS PREDICTED BY USER FROM CS122DIESELHC/2.0/
Parameter SGDIESELHC,SULDIESELHC/.03/,FLSHDIESELHC/200/,PORDIESELHC/-50/
        CETDIESELHC/62/,CS122DIESELHC/2.0/,CS210DIESELHC/1.2/,V650DIESELHC/90/;
SGDIESELHC= (600+460)**.3333/KDslHC;

*Volumetric Flowrates
Variable FLNHC,FHNHC,FKEROHC,FDIESELHC;
Equation RATEVLNHC1,RATEVHNHC1,RATEVKEROHC1,RATEVDIESELHC1;
RATEVDIESELHC1.. FDIESELHC=E=RATEWDIESELHC/(SGDIESELHC*0.3502);

*  UTILITIES
Variable
GasLHVHC,FuelHC,NOXHC,NOXHC2,NOXHC3,PowerHC,CWHC,CHEMHC,CapitalHC;
Equation
GasLHVHC1,FuelHC1,NOXHC1,NOXHC22,NOXHC33,PowerHC1,CWHC1,CHEMHC1,Capit
alHC1;
GasLHVHC1..  GasLHVHC =E=GasHC*21;
FuelHC1..    FuelHC   =E= -RateVHC*(.09+.03*ModeHC);
NOXHC1..     NOXHC =E= EF*(-FuelHC);
NOXHC22..    NOXHC2 =E= EF2*(-FuelHC);
```

```
NOXHC33..    NOXHC3 =E= EF3*(-FuelHC);

PowerHC1..    PowerHC  =E= -RateVHC*(3+4*ModeHC);

CWHC1..       CWHC     =E= -RateVHC*0.33;

ChemHC1..     ChemHC   =E= -RateVHC*(.1*ModeHC+.003*(NIHC+VANHC));

CapitalHC1.. CapitalHC=E= (-
94*(RateVHC/30000)**.65)*((SCFHYDHC/1600)**.4)*(((NIHC+VANHC+30)/30)**.2);

BINARY VARIABLE X1HC,X2HC,X3HC;

VARIABLE TNOXHC;

EQUATION Q16,QQ16,QQQ16;

Q16..  TNOXHC =E= X1HC*NOXHC+X2HC*NOXHC2;

QQ16..  X2HC+X3HC =L= 1;

QQQ16.. X1HC+X2HC =E= 1;


*-------------------------------------------------------------------

*---------------------------------------------------------------------

*  FCC.mod

* Products: FCCLN, FCCHN, LCO, SlurryOil, Coke

* Parameters: Conv(75),LNEP(250),HNEP(430)

*             Note that Conv is Wt% conversion (100 minus percent 430F+)

*             and LN,HN End points (must be DegF)

* User entered end points must not be too far from default values to maintain accuracy.

* Feed Properties used:   Con Carbon,VABP,VAN,NI


* Feed Rate and Properties

*Parameter SGFCC,APIFCC,VABPFCC,SULFCC,NIFCC,VANFCC,CCRFCC;

*Variable RateWFCC,RateVFCC;
```

```
*Equation RateWFCC1,RateVFCC1;

*RATEVFCC1.. RATEVFCC=E= FTGOFCC;

*RATEWFCC1.. RATEWFCC=E= RATEVFCC*SGFCC*0.3502;

*SGFCC   = SGTGO;

*APIFCC  = 141.5/SGFCC-131.5;

*VABPFCC = VABPTGO;

*CCRFCC  = CCRTGO;

*NIFCC   = NITGO;

*VANFCC  = VANTGO;

*SULFCC  = SULTGO;


*YIELDS

* First pass wt frac yields - have suffix a

*Parameter CONVFCC/75/

*          LNEPFCC/250/

*         HNEPFCC/430/;

*Parameter KPFCC,CokeaFCC,GasaFCC,H2SaFCC,LPGaFCC,LCOaFCC,SLRYaFCC

*         NAPHaFCC      Total C5-430F cut naphtha

*         LNaFCC        C5-160F light naphtha

*         Inter1HNFCC    160-260 naphtha. Will be split and merged above-below

*         HNaFCC        260-360 heavy naphtha

*         Inter2LCOFCC    360-430 naphtha. Will be split and merged above-below;

*Equation KPFCC1,CokeaFCC1,GasaFCC1,H2SaFCC1,LPGaFCC1,LCOaFCC1,SLRYaFCC1

*         NAPHaFCC1,LNaFCC1,Inter1HNFCC1,HNaFCC1,Inter2LCOFCC1;

*KPFCC     = 1.6667*(VABPFCC+460)**0.3333/SGFCC-19.67;
```

```
*LPGaFCC   = -.0279+.000839*CONVFCC+.00002343*CONVFCC**2 + KPFCC*(-
.1067+.003724*CONVFCC-.00003419*CONVFCC**2);

*NAPHaFCC  = CONVFCC/100-CokeaFCC-GasaFCC-H2SaFCC-LPGaFCC;

*LCOaFCC   = (0.7+(CONVFCC-75)*.005)*(1-CONVFCC/100);

*SLRYaFCC  =1-CONVFCC/100-LCOaFCC;

*LNaFCC    = NaphaFCC*(.29+(CONVFCC-75)*.005);

*Inter1HNFCC= NaphaFCC*0.265;

*HNaFCC    = NaphaFCC*0.275;

*Inter2LCOFCC= NaphaFCC-LNaFCC-Inter1HNFCC-HNaFCC;


* Final pass wt frac yields to account for LN,HN,LCGO endpoints entered by user

* Intermediate cut Inter12 is split and light portion will merge with LN, hvy portion with HN

*Parameter Light1HNFCC Light12 will be merged with LN

*        Heavy1HNFCC  Heavy12 will be merged with HN

*        Light2LCOFCC  Light23 will be merged with HN

*        Heavy2LCOFCC  Heavy23 will be merged with LCO

*       LNbFCC      Light Naphtha

*        HNbFCC      Heavy Naphtha

*        LCObFCC     Light C Oil;


*Equation
Light1HNFCC1,Heavy1HNFCC1,Light2LCOFCC1,Heavy2LCOFCC1,LNbFCC1,HNbFCC1,L
CObFCC1;

*Light1HNFCC=Inter1HNFCC *(LNEPFCC-160)/100;

*Heavy1HNFCC=Inter1HNFCC -Light1HNFCC;

*Light2LCOFCC=Inter2LCOFCC *(HNEPFCC-360)/70;

*Heavy2LCOFCC=Inter2LCOFCC -Light2LCOFCC;
```

```
* These are final weight fraction yields after merging the swing cuts into the four liquid products

*LNbFCC = LNaFCC + Light1HNFCC;

*HNbFCC = Heavy1HNFCC + HNaFCC + Light2LCOFCC;

*LCObFCC= Heavy2LCOFCC + LCOaFCC;


* Final weight rates from wt frac yields

*Variable H2SFCC,GasFCC,C3UFCC,C3SFCC,IC4FCC,NC4FCC,IC4UFCC,C4UFCC

*        RateWLNFCC,RateWHNFCC,RateWLCOFCC,RateWHCOFCC,RateW5FCC;

*Equation
H2SFCC1,GasFCC1,C3UFCC1,C3SFCC1,IC4FCC1,NC4FCC1,IC4UFCC1,C4UFCC1

*        RateWLNFCC1,RateWHNFCC1,RateWLCOFCC1,RateWHCOFCC1,RateW5FCC1;

*H2SFCC1..    H2SFCC   =E=RateWFCC*H2SaFCC;

*GasFCC1..    GasFCC   =E=RateWFCC*GasaFCC;

*C3UFCC1..    C3UFCC   =E=0.25*RateWFCC*LPGaFCC;

*C3SFCC1..    C3SFCC   =E=0.09*RateWFCC*LPGaFCC;

*IC4FCC1..    IC4FCC   =E=0.21*RateWFCC*LPGaFCC;

*NC4FCC1..    NC4FCC   =E=0.07*RateWFCC*LPGaFCC;

*IC4UFCC1..   IC4UFCC  =E=0.15*RateWFCC*LPGaFCC;

*C4UFCC1..    C4UFCC   =E=0.23*RateWFCC*LPGaFCC;

*RateWLNFCC1.. RateWLNFCC=E=RateWFCC*LNbFCC;

*RateWHNFCC1.. RateWHNFCC=E=RateWFCC*HNbFCC;

*RateWLCOFCC1.. RateWLCOFCC=E=RateWFCC*LCObFCC;

*RateWHCOFCC1.. RateWHCOFCC=E=RateWFCC*SLRYaFCC;

*RateW5FCC1.. RateW5FCC=E=RateWFCC*CokeaFCC;
```

```
*API Gravities

*Parameter SG5FCC Coke (Ficticious SG to give zero liquid yld)

*        APILNFCC,APIHNFCC,APILCOFCC,APIHCOFCC

*        SGLNFCC,SGHNFCC,SGLCOFCC,SGHCOFCC;

*SG5FCC = 10**20;

*APILCOFCC= ((41+KPFCC*6)*Heavy2LCOFCC +(20+KPFCC*5+(75-
CONVFCC)*0.2)*LCOaFCC)/LCObFCC;

*APIHCOFCC= 2+KPFCC*6+(75-CONVFCC)*0.2;

*SGLNFCC = 141.5/(APILNFCC+131.5);

*SGHNFCC = 141.5/(APIHNFCC+131.5);

*SGLCOFCC= 141.5/(APILCOFCC+131.5);

*SGHCOFCC= 141.5/(APIHCOFCC+131.5);


*Sulfur

*Parameter SulLNFCC,SulHNFCC,SulLCOFCC,SulHCOFCC;

*SulLNFCC = SULFCC*(0.01*LNaFCC +0.05*Light1HNFCC)/LNbFCC;

*SulHNFCC = SULFCC*(0.05*Heavy1HNFCC +0.08*HNaFCC +0.12*Light2LCOFCC)
/HNbFCC;

*SulLCOFCC= SULFCC*(0.12*Heavy2LCOFCC +1.3*LCOaFCC)/LCObFCC;

*SulHCOFCC= SULFCC*2.5;


* OTHER PROPERTIES (LNaph, HNaph & LCO)


*Parameter RVPLNFCC/10/,V300LNFCC/100/,V400LNFCC/100/

*         RVPHNFCC/4/,FRZHNFCC/-10/,SMKHNFCC/10/,V150HNFCC/0/
```

```
*        PORLCOFCC/5/,CETLCOFCC/25/,FRZLCOFCC/-5/,CS122LCOFCC/2.2/,CS210LCOFCC/1.1/,SMKLCOFCC/10/,OLELCOFCC/30/,AROLCOFCC/40/
* PORHCOFCC/50/,VABPHCOFCC/1000/,FLSHHCOFCC/260/,CS122HCOFCC/30/,CS210HCOFCC/6/,CCRHCOFCC/30/;
*Parameter RONLNFCC,MONLNFCC,OLELNFCC,AROLNFCC,V150LNFCC,V200LNFCC
* RONHNFCC,MONHNFCC,OLEHNFCC,AROHNFCC,V200HNFCC,V300HNFCC,V400HNFCC
*        FLSHLCOFCC,V500LCOFCC,V650LCOFCC,VABPLCOFCC;
* LNaph
*RONLNFCC =(90*LNaFCC +93*Light1HNFCC)/LNbFCC;
*MONLNFCC =RONLNFCC-10.5;
*OLELNFCC =(40*LNaFCC +30*Light1HNFCC)/LNbFCC;
*AROLNFCC =30*Light1HNFCC/LNbFCC;
*V150LNFCC=90*LNaFCC/LNbFCC;
*V200LNFCC=(100*LNaFCC+40*Light1HNFCC)/LNbFCC;

* HNaph
*AROHNFCC =(30*Heavy1HNFCC +35*HNaFCC +40*Light2LCOFCC)/HNbFCC;
*V200HNFCC=60*Heavy1HNFCC/HNbFCC;
*V300HNFCC=(100*Heavy1HNFCC +40*HNaFCC)/HNbFCC;
*V400HNFCC=(100*Heavy1HNFCC +100*HNaFCC +65*Light2LCOFCC)/HNbFCC;

* LCO
*FLSHLCOFCC=(150*Heavy2LCOFCC +210*LCOaFCC)/LCObFCC;
*V500LCOFCC=(100*Heavy2LCOFCC +LCOaFCC*40)/LCObFCC;
```

```
* Products: Reformate

* Parameters: Severity(100), Pressure(150)

* Note that Severity is product RON and Pressure must be psia (range 30-500)

* Feed Properties: NAPH, ARO, V150, V300, V400


*Feed Rate and Properties

Variable
RATEVREF,SGREF,RATEWREF,NAPHREF,AROREF,V150REF,V200REF,V300REF,V400REF;

Equation
RATEVREF1,SGREF1,RATEWREF1,NAPHREF1,AROREF1,V150REF1,V200REF1,V300REF1,V400REF1;

RATEVREF1.. RATEVREF =E= FTHN + FNDHT + FNGOHT + FNRDHT +FHNHC;

SGREF1..    SGREF*RATEVREF =E=
FTHN*SGTHN+FNDHT*SGNDHT+FNGOHT*SGNGOHT+FNRDHT*SGNRDHT
+FHNHC*SGHNHC;

RATEWREF1.. RATEWREF =E= RATEVREF*SGREF*0.3502;

NAPHREF1..  NAPHREF*RATEVREF=E=
FTHN*NAPHTHN+FNDHT*NAPHNDHT+FNGOHT*NAPHNGOHT+FNRDHT*NAPHNRDHT+FHNHC*NAPHHNHC;

AROREF1..   AROREF *RATEVREF=E= FTHN*AROTHN +FNDHT*ARONDHT
+FNGOHT*ARONGOHT +FNRDHT*ARONRDHT +FHNHC*AROHNHC;

V150REF1..  V150REF*RATEVREF=E=
FTHN*V150THN+FNDHT*V150NDHT+FNGOHT*V150NGOHT+FNRDHT*V150NRDHT+
FHNHC*V150HNHC;

V200REF1..  V200REF*RATEVREF=E=
FTHN*V200THN+FNDHT*V200NDHT+FNGOHT*V200NGOHT+FNRDHT*V200NRDHT+
FHNHC*V200HNHC;

V300REF1..  V300REF*RATEVREF=E=
FTHN*V300THN+FNDHT*V300NDHT+FNGOHT*V300NGOHT+FNRDHT*V300NRDHT+
FHNHC*V300HNHC;
```

```
V400REF1..  V400REF*RATEVREF=E=
FTHN*V400THN+FNDHT*V400NDHT+FNGOHT*V400NGOHT+FNRDHT*V400NRDHT+
FHNHC*V400HNHC;


* YIELDS

Parameter SEVERITYREF/100/

        PressureREF psia/150/;

Variable LVYLDREF,H2REF,GASREF,C3SREF,IC4REF,NC4REF,RATEW1REF;

Equation LVYLDREF1,H2REF1,GASREF1,C3SREF1,IC4REF1,NC4REF1,RATEW1REF1;

LVyldREF1..  LVyldREF =E=81.8-0.035*(PressureREF-50)+0.2*(NAPHREF+2*AROREF-39)-
1.0*(SeverityREF-100);

H2REF1..     H2REF*100=E=RateWREF*(3.2-.0118*(PressureREF-50)-0.2*(LVyldREF-81.8));

*SCFHYDREF1.. SCFHYDREF=E=(3.2-.0118*(PressureREF-50)-0.2*(LVyldREF-
81.8))*658*SGREF;

GasREF1..    GasREF   =E=RateWREF*(2.2-0.19*(LVyldREF-81.8))/100;

C3SREF1..    C3SREF   =E=RateWREF*(2.0-0.2*(LVyldREF-81.8))/100;

IC4REF1..    IC4REF   =E=RateWREF*(1.3-.055*(LVyldREF-81.8))/100;

NC4REF1..    NC4REF   =E=IC4REF*58/42;

RateW1REF1.. RateW1REF=E=RateWREF-H2REF-GasREF-C3SREF-IC4REF-NC4REF;


* Products properties

* Reformate

RONREFORMAT =SeverityREF;

MONREFORMAT =RONREFORMAT-9;

Variable
SGREFORMAT,FREFORMATE,BENZREFORMAT,V150REFORMAT,V200REFORMAT,V3
00REFORMAT,V400REFORMAT;
```

```
Equation
SG1REFORMAT,RATEV1REFORMAT,BENZ1REFORMAT,V1501REFORMAT,V2001REFORMAT,V3001REFORMAT,V4001REFORMAT;

SG1REFORMAT..    SGREFORMAT  =E=RateW1REF/(RateVREF*LVyldREF*0.3502/100);

RATEV1REFORMAT.. FREFORMATE  =E=RATEW1REF/(SGREFORMAT*0.3502);

BENZ1REFORMAT..  BENZREFORMAT=E=(V200REF-V150REF)*0.5*(1+(SeverityREF-100)*.12);

V1501REFORMAT..  V150REFORMAT=E=V150REF;

V2001REFORMAT..  V200REFORMAT=E=V200REF;

V3001REFORMAT..  V300REFORMAT=E=V300REF;

V4001REFORMAT..  V400REFORMAT=E=V400REF;


*   UTILITIES

Variable
FUELREF,HPSREF,BFWREF,POWERREF,CWREF,GASLHVREF,CAPITALREF,NOXREF,NOXREF2,NOXREF3;

Equation
FUELREF1,HPSREF1,BFWREF1,POWERREF1,CWREF1,GASLHVREF1,CAPITALREF1,NOXREF1,NOXREF22,NOXREF33;

FuelREF1..    FuelREF   =E= -RateVREF*.258;

HPSREF1..     HPSREF    =E= RateVREF*.1;

BFWREF1..     BFWREF    =E= -HPSREF;

PowerREF1..   PowerREF  =E= -RateVREF*1.0;

CWREF1..      CWREF     =E= -RateVREF*0.6;

GasLHVREF1..  GasLHVREF =E= GasREF*21;

CapitalREF1.. CapitalREF=E= -48*(1-.0012*(PressureREF-50))*(RateVREF/20000)**0.65;

NOXREF1..

NOXREF22..

NOXREF33..
```

```
BINARY VARIABLE X1REF,X2REF,X3REF;
VARIABLE TNOXREF;
EQUATION Q18,QQ18,QQQ18;
Q18..  TNOXREF =E= X1REF*NOXREF+X2REF*NOXREF2;
QQ18..
QQQ18.. X1REF+X2REF =E= 1;


*-----------------------------------------------------------------------
*------------------------------------------------------------------------
* BLENDING



Variable Z,FGASOLINE,FKEROSENE,FDSL,FFOIL;
PARAMETER perred/0.0/;
POSITIVE VARIABLE NOXTC;
*BINARY VARIABLE Y;
EQUATION NOXTOT1,Q2;
NOXTOT1..  NOXTC=E=1*((TNOXCDU+TNOXRDHT+TNOXVis +TNOXHC+TNOXREF)-
(X3CDU*NOXCDU+X3RDHT*NOXRDHT+X3Vis*NOXVis+X3GOHT*NOXGOHT
+X3REF*NOXREF));
Q2..      NOXTC=L=(1-perred)*26437.0;


Equation Obj,MOGAS,KERO,DIESEL,FUELOIL,Dem1,Dem2,Dem3,Dem4;
* The Gases of all units can be seperated on GAS PLANT into MixC3 & MixC4
* MixC3 = 2160 & MixC4 =  4470 Barrel
* C3 & C4 price are 35.7 & 39.9, respectively
```

```
Obj..   Z=E= (1*(1.0*(108*FGASOLINE +86*FKEROSENE +120*FDSL +66*FFOIL) -
70*100000)+1*(-X1CDU*COST1-X2CDU*COST2CDU-X3CDU*COST3CDU

-X1RDHT*COST1-X2RDHT*COST2RDHT-X3RDHT*COST3RDHT-X1Vis*Cost1-
X2Vis*Cost2Vis-X3Vis*Cost3Vis-X1GOHT*COST1-X2GOHT*COST2GOHT-
X3GOHT*COST3GOHT-X1DHT*COST1-X2DHT*COST2DHT-X3DHT*COST3DHT

-X1NHT*COST1-X2NHT*COST2NHT-X3NHT*COST3NHT-X1HC*COST1-
X2HC*COST2HC-X3HC*COST3HC-X1REF*COST1-X2REF*COST2REF-
X3REF*COST3REF))*1;

* The Gases of all units can be seperated on GAS PLANT into MixC3 & MixC4

* MixC3 = 2160 & MixC4 =  4470 Barrel

* C3 & C4 price are 35.7 & 39.9, respectively

MOGAS..   FGASOLINE =E= RateV1Vis+FLSRN+FTLN+FREFORMATE+FLNHC;

KERO..    FKEROSENE =E= FKERO+FKDHTK+FKEROHC;


Positive Variable
SGGASOLINE,SULGASOLINE,RONGASOLINE,RVPGASOLINE,V150GASOLINE,V200G
ASOLINE,V300GASOLINE,V400GASOLINE

         SGKEROSENE,SULKEROSENE,SMKKEROSENE,FLSHKEROSENE

         SGDSL,SULDSL,CETDSL,CS122DSL,FLSHDSL

         SGFOIL,SULFOIL,CS122FOIL;

Negative Variable FRZKEROSENE;

Equation
SGMOGAS,SULMOGAS,RONMOGAS,RVPMOGAS,V150MOGAS,V200MOGAS,V300MO
GAS,V400MOGAS

         SGKERO,SULKERO,SMKKERO,FLSHKERO,FRZKERO

         SGDIESEL1,SULDIESEL1,CETDIESEL1,CS122DIESEL1,FLSHDIESEL1

         SGFUELOIL1,SULFUELOIL1,CS122FUELOIL1;

* Gasoline properties

SGMOGAS..   FGASOLINE*SGGASOLINE  =E=
FLSRN*LSRSG+FTLN*SGTLN+FREFORMATE*SGREFORMAT+FLNHC*SGLNHC;
```

```
SULMOGAS..  (FGASOLINE*SGGASOLINE*0.3502)*SULGASOLINE =E=
RATEWLSRN*LSRS;

RONMOGAS..  FGASOLINE*RONGASOLINE =E=
FLSRN*RON2+FTLN*RONTLN+FREFORMATE*RONREFORMAT+FLNHC*RONLNHC;

*MONMOGAS..  FGASOLINE*MONGASOLINE =E=
FLSRN*MON2+FTLN*MONTLN+FREFORMATE*MONREFORMAT+FLNHC*MONLNHC
+FLNFCC*MONLNFCC+FHNFCC*MONHNFCC;

RVPMOGAS..  FGASOLINE*RVPGASOLINE**1.25 =E=
FLSRN*(RVP2**1.25)+FTLN*(RVPTLN**1.25)+FREFORMATE*(RVPREFORMAT**1.25)
+FLNHC*(RVPLNHC**1.25);

V150MOGAS.. FGASOLINE*V150GASOLINE=E=
FLSRN*V1502+FTLN*V150TLN+FREFORMATE*V150REFORMAT+FLNHC*V150LNHC;

V200MOGAS.. FGASOLINE*V200GASOLINE=E=
FLSRN*V2002+FTLN*V200TLN+FREFORMATE*V200REFORMAT+FLNHC*V200LNHC;

V300MOGAS.. FGASOLINE*V300GASOLINE=E=
FLSRN*V3002+FTLN*V300TLN+FREFORMATE*V300REFORMAT+FLNHC*V300LNHC;

V400MOGAS.. FGASOLINE*V400GASOLINE=E=
FLSRN*V4002+FTLN*V400TLN+FREFORMATE*V400REFORMAT+FLNHC*V400LNHC;


FRZKERO..  FKEROSENE*Exp(13.333*LOG((FRZKEROSENE+460)/600))=E=
FKERO*Exp(13.333*LOG((FRZ4+460)/600))+FKDHTK*Exp(13.333*LOG((FRZKDHT+460)/
600))+FKEROHC*Exp(13.333*LOG((FRZKEROHC+460)/600));

* V300KERO.. FKEROSENE* =E=
FKERO*V3004+FKDHTK*V300KDHT+FKEROHC*V300??;

* V400KERO.. FKEROSENE* =E=
FKERO*V4004+FKDHTK*V400KDHT+FKEROHC*V400??;

* V500KERO.. FKEROSENE* =E=
FKERO*V5004+FKDHTK*V500KDHT+FKEROHC*V500??;


* Diesel properties

SGDIESEL1..    FDSL*SGDSL
=E=FTDIESEL*SGDDHT+FDRDHTD*SGDRDHT+FDGOHTD*SGDGOHT+FKDHTD*SGK
DHT+FDIESELHC*SGDIESELHC;
```

```
SULDIESEL1..   (FDSL*SGDSL*0.3502)*SULDSL =E=RATEW3DHT*SULDDHT+RATEW2RDHT*SULDRDHT+RATEW2GOHT*SULDGOHT+RATEW2DHT*SULKDHT+RATEWDIESELHC*SULDIESELHC;

CETDIESEL1..   FDSL*CETDSL =E=FTDIESEL*CETDDHT+FDRDHTD*CETDRDHT+FDGOHTD*CETDGOHT+FKDHTD*CETKDHT+FDIESELHC*CETDIESELHC;

CS122DIESEL1.. FDSL*LOG(LOG(CS122DSL+0.8))=E=FTDIESEL*(LOG(LOG(CS122DDHT+0.8)))+FDRDHTD*(LOG(LOG(CS122DRDHT+0.8)))+FDGOHTD*(LOG(LOG(CS122DGOHT+0.8)))+FKDHTD*(LOG(LOG(CS122KDHT+0.8)))+FDIESELHC*(LOG(LOG(CS122DIESELHC+0.8)));

*CS210DIESEL1.. FDSL*LOG(LOG(CS210DSL+0.8))=E=FTDIESEL*(LOG(LOG(CS210DDHT+0.8)))+FDRDHTD*(LOG(LOG(CS210DRDHT+0.8)))+FDGOHTD*(LOG(LOG(CS210DGOHT+0.8)))+FKDHTD*(LOG(LOG(CS210KDHT+0.8)))+FLCOFCC*(LOG(LOG(CS210LCOFCC+0.8)))+FDIESELHC*(LOG(LOG(CS210DIESELHC+0.8)));

*ARODIESEL1..   FDSL*   =E= FTDIESEL*ARODDHT+FDRDHTD*?????+FDGOHTD*ARODGOHT+FKDHTD*AROKDHT+FLCOFCC*AROLCOFCC+FDIESELHC*;

FLSHDIESEL1..  FDSL*EXP(-16.667*LOG((FLSHDSL+460)/600))=E=FTDIESEL*(EXP(-16.667*LOG((FLSHDDHT+460)/600)))+FDRDHTD*(EXP(-16.667*LOG((FLSHDRDHT+460)/600)))+FDGOHTD*(EXP(-16.667*LOG((FLSHDGOHT+460)/600)))+FKDHTD*(EXP(-16.667*LOG((FLSHKDHT+460)/600)))+FDIESELHC*(EXP(-16.667*LOG((FLSHDIESELHC+460)/600)));


* FuelOil properties

SGFUELOIL1..    FFOIL*SGFOIL   =E= FLSFO*SGLSFO+FDRDHTF*SGDRDHT+FDGOHTF*SGDGOHT;

SULFUELOIL1..   FFOIL*SULFOIL  =E= RATEW3RDHT*SULLSFO+RATEW2RDHT*SULDRDHT+RATEW2GOHT*SULDGOHT;

CS122FUELOIL1.. FFOIL*LOG(LOG(CS122FOIL+0.8))=E= FLSFO*(LOG(LOG(CS122LSFO+0.8)))+FDRDHTF*(LOG(LOG(CS122DRDHT+0.8)))+FDGOHTF*(LOG(LOG(CS122DGOHT+0.8)));
```

```
*CS210FUELOIL1.. FFOIL*LOG(LOG(CS210FOIL+0.8))=E=
FLSFO*(LOG(LOG(CS210LSFO+0.8)))+FDRDHTF*(LOG(LOG(CS210DRDHT+0.8)))+FDG
OHTF*(LOG(LOG(CS210DGOHT+0.8)))+FHCOFCC*(LOG(LOG(CS210HCOFCC+0.8)));


Equation pro1,pro2,pro3,pro5,pro6,pro7,pro8,pro9,pro10,pro11,pro13

         pro14,pro15,pro16,pro17,pro18,pro19,pro21,pro22,pro23,pro24;

PRO1..  SGGASOLINE   =L=0.817;

PRO2..  SULGASOLINE  =L=0.05;

PRO3..  RONGASOLINE  =G=89;

*PRO4..  MONGASOLINE  =G=

PRO5..  RVPGASOLINE  =L=9.0;

PRO6..  V150GASOLINE =G=10;

PRO7..  V200GASOLINE =G=27.5;

PRO8..  V300GASOLINE =G=60;

PRO9..  V400GASOLINE =G=92.5;

PRO10.. SGKEROSENE   =L=0.85;

PRO11.. SULKEROSENE  =L=0.25;

*PRO12.. AROKEROSENE =G=

PRO13.. SMKKEROSENE  =G=20;

PRO14.. FLSHKEROSENE =G=136;

PRO15.. FRZKEROSENE  =G=-50;

PRO16.. SGDSL        =L=0.875;

PRO17.. SULDSL       =L=0.5;

PRO18.. CETDSL       =G=45;

PRO19.. CS122DSL     =L=5.5;

*PRO20.. CS210DSL     =L=
```

```
PRO21.. FLSHDSL      =G= 130;
PRO22.. SGFOIL       =L=1.0;
PRO23.. SULFOIL      =L=1.0;
PRO24.. CS122FOIL    =L=5.0E+06;
*PRO25.. CS210FOIL    =L=

*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
* Lower & upper limits and Initial values of the final properties

*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
* Lower & upper limits and Initial values of the streams and units variables

* FINAL FLOWRATE variables Lower & upeer limits
FGASOLINE.lo=0   ; FGASOLINE.up=40000    ; FGASOLINE.l=31170     ;
FKEROSENE.lo=0   ; FKEROSENE.up=40000    ; FKEROSENE.l=23600     ;
FDSL.lo=0        ; FDSL.up=40000         ; FDSL.l=25800          ;
FFOIL.lo=0       ; FFOIL.up=40000        ; FFOIL.l=16200         ;
FREFORMATE.lo=0  ; FREFORMATE.up=20000   ; FREFORMATE.l=15000    ;
FDRDHTD.lo=0     ; FDRDHTD.up=2000       ; FDRDHTD.l=1310        ;
FDRDHTF.lo=0     ; FDRDHTF.up=2000       ; FDRDHTF.l=0           ;
FDGOHTD.lo=0     ; FDGOHTD.up=2500       ; FDGOHTD.l=1440        ;
FDGOHTF.lo=0     ; FDGOHTF.up=1500       ; FDGOHTF.l=0           ;
FKDHTK.lo=0      ; FKDHTK.up=13000       ; FKDHTK.l=2160         ;
FKDHTD.lo=0      ; FKDHTD.up=13000       ; FKDHTD.l=5            ;
```

```
RateWHNHC.lo=0   ; RateWHNHC.up=1000     ; RateWHNHC.l=416       ;
RateWKEROHC.lo=0 ; RateWKEROHC.up=4000   ; RateWKEROHC.l=2885    ;
RateWDIESELHC.lo=0;RateWDIESELHC.up=4000 ; RateWDIESELHC.l=3148  ;
GasLHVHC.lo=0    ; GasLHVHC.up=10000     ; GasLHVHC.l=850        ;
FuelHC.lo=-2500  ; FuelHC.up=0           ; FuelHC.l=-1900        ;
CHEMHC.lo=-5000  ; CHEMHC.up=0           ; CHEMHC.l=-1600        ;
PowerHC.lo=-150000; PowerHC.up=0         ; PowerHC.l=-110000     ;
CWHC.lo=-10000   ; CWHC.up=0             ; CWHC.l=-5200          ;
CapitalHC.lo=-100; CapitalHC.up=0        ; CapitalHC.l=-66       ;

*FCC variables Lower & upeer limits
*RateVFCC.lo=10000; RateVFCC.up=25000     ; RateVFCC.l=10433      ;
*RateWFCC.lo=3000 ; RateWFCC.up=7000      ; RateWFCC.l=3358       ;
*H2SFCC.lo=0      ; H2SFCC.up=10          ; H2SFCC.l=1            ;
*GasFCC.lo=0      ; GasFCC.up=300         ; GasFCC.l=122          ;
*C3UFCC.lo=0      ; C3UFCC.up=400         ; C3UFCC.l=200          ;
*C3SFCC.lo=-20    ; C3SFCC.up=200         ; C3SFCC.l=70           ;
*IC4FCC.lo=-20    ; IC4FCC.up=400         ; IC4FCC.l=165          ;
*IC4UFCC.lo=-20   ; IC4UFCC.up=300        ; IC4UFCC.l=118         ;
*NC4FCC.lo=-20    ; NC4FCC.up=100         ; NC4FCC.l=55           ;
*C4UFCC.lo=0      ; C4UFCC.up=200         ; C4UFCC.l=181          ;
*RateWLNFCC.lo=0  ; RateWLNFCC.up=2000    ; RateWLNFCC.l=5650     ;
*RateWHNFCC.lo=0  ; RateWHNFCC.up=5000    ; RateWHNFCC.l=4550     ;
*RateWLCOFCC.lo=0 ; RateWLCOFCC.up=2000   ; RateWLCOFCC.l=2800    ;
*RateWHCOFCC.lo=0 ; RateWHCOFCC.up=5000   ; RateWHCOFCC.l=1060    ;
*RateW5FCC.lo=0   ; RateW5FCC.up=5000     ;
```

```
*GasLHVFCC.lo=0   ; GasLHVFCC.up=10000    ; GasLHVFCC.l=2600      ;

*HPSFCC.lo=0      ; HPSFCC.up=1000        ; HPSFCC.l=475          ;

*CHEMFCC.lo=-5000 ; CHEMFCC.up=0          ; CHEMFCC.l=-1600       ;

*PowerFCC.lo=-150000; PowerFCC.up=0       ; PowerFCC.l=-95000     ;

*BFWFCC.lo=-1000  ; BFWFCC.up=0           ; BFWFCC.l=-475         ;

*CWFCC.lo=-10000  ; CWFCC.up=0            ; CWFCC.l=-8000         ;

*CapitalFCC.lo=-100; CapitalFCC.up=0      ; CapitalFCC.l=-56      ;


*Reformer variables Lower & upeer limits

RateVREF.lo=0    ; RateVREF.up=29000     ; RateVREF.l=18020      ;

SGREF.lo=0       ; SGREF.up=1.0          ; SGREF.l=0.7829        ;

RateWREF.lo=0    ; RateWREF.up=5500      ; RateWREF.l=4940       ;

AROREF.lo=0      ; AROREF.up=100         ; AROREF.l=18.0         ;

NAPHREF.lo=0     ; NAPHREF.up=50         ; NAPHREF.l=30.8        ;

V150REF.lo=0     ; V150REF.up=100        ; V150REF.l=0.5         ;

V200REF.lo=0     ; V200REF.up=100        ; V200REF.l=9.1         ;

V300REF.lo=0     ; V300REF.up=100        ; V300REF.l=52.6        ;

V400REF.lo=0     ; V400REF.up=100        ; V400REF.l=92.5        ;

LVYLDREF.lo=0    ; LVYLDREF.up=100       ; LVYLDREF.l=83.98      ;

H2REF.lo=0       ; H2REF.up=200          ; H2REF.l=79            ;

GasREF.lo=0      ; GASREF.up=200         ; GASREF.l=89           ;

C3SREF.lo=0      ; C3SREF.up=200         ; C3SREF.l=78           ;

IC4REF.lo=0      ; IC4REF.up=200         ; IC4REF.l=58           ;

NC4REF.lo=0      ; NC4REF.up=200         ; NC4REF.l=81           ;

RateW1REF.lo=0   ; RateW1REF.up=5500     ; RateW1REF.l=4546      ;

SGREFORMAT.lo=0  ; SGREFORMAT.up=1.0     ; SGREFORMAT.l=.861     ;
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```
BENZREFORMAT.lo=0; BENZREFORMAT.up=100   ; BENZREFORMAT.l=4.5    ;
V150REFORMAT.lo=0; V150REFORMAT.up=100   ; V150REFORMAT.l=0.5    ;
V200REFORMAT.lo=0; V200REFORMAT.up=100   ; V200REFORMAT.l=9.1    ;
V300REFORMAT.lo=0; V300REFORMAT.up=100   ; V300REFORMAT.l=52.6   ;
V400REFORMAT.lo=0; v400REFORMAT.up=100   ; v400REFORMAT.l=92.5   ;
FuelREF.lo=-9000 ; FuelREF.up=0          ; FuelREF.l=-4548       ;
HPSREF.lo=0      ; HPSREF.up=5000        ; HPSREF.l=1763         ;
BFWREF.lo=-5000  ; BFWREF.up=0           ; BFWREF.l=-1763        ;
PowerREF.lo=-50000; PowerREF.up=0        ; PowerREF.l=-17630     ;
CWREF.lo=-25000  ; CWREF.up=0            ; CWREF.l=-10580        ;
GasLHVREF.lo=0   ; GasLHVREF.up=8000     ; GasLHVREF.l=1810      ;
CapitalREF.lo=-100; CapitalREF.up=0      ; CapitalREF.l=-39      ;


Model Basic /all/;
Solve Basic maximizing Z using minlp;
Display
NOXCDU,NOXCDU2,NOXCDU3,NOXRDHT,NOXRDHT2,NOXRDHT3,NOXVis,NOXVis2,
NOXVis3,NOXGOHT,
NOXGOHT2,NOXGOHT3,NOXDHT,NOXDHT2,NOXDHT3,NOXNHT,NOXNHT2,NOXNH
T3,NOXHC.l,NOXHC2.l,NOXHC3.l,
NOXREF.l,NOXREF2.l,NOXREF3.l,NOXTC.l;
DISPLAY
X1CDU.L,X2CDU.L,X3CDU.L,X1RDHT.L,X2RDHT.L,X3RDHT.L,X1Vis.l,X2Vis.l,X3Vis.l,
X1GOHT.L,X2GOHT.L,X3GOHT.L,
X1DHT.L,X2DHT.L,X3DHT.L,X1NHT.L,X2NHT.L,X3NHT.L,X1HC.L,X2HC.L,X3HC.L,
X1REF.L,X2REF.L,X3REF.L;


Display FLPG,FLSRN,FHSRN,FKERO,FDIESEL,FLVGO,FHVGO,FRSD;
```

```
Display RateVHC.l;
Display FGASOLINE.l,FKEROSENE.l,FDSL.l,FFOIL.l;
Display FLSRN,FTLN,FREFORMATE.L,FLNHC.L;
Display FKERO,FKDHTK.L,FKEROHC.L;
Display FTDIESEL,FDRDHTD.L,FDGOHTD.L,FKDHTD.L,FDIESELHC.L;
Display FLSFO,FDRDHTF.L,FDGOHTF.L;
Display SGDSL.L,SULDSL.L,CETDSL.L,CS122DSL.L,FLSHDSL.L;
Display SGFOIL.L,SULFOIL.L,CS122FOIL.L;
```

Nomenclature

CDU-Crude Distillation Unit

LPG-Liquefied Petroleum Gas

LSR-Light Straight Run

HSR-Heavy Straight Run

VDU- Vacuum Distillation Unit

H/C –Hydrocarbons

CCR- Continuous Catalyst Regeneration

LP-Linear Programming

MILP-Mixed Integer Linear Programming

MINLP-Mixed Integer Non Linear Programming

NAAQS-National Ambient Air Quality Standard

SCR-Selective Catalytic Reduction

SNCR-Selective Non-Catalytic Reduction

DEF-Diesel Exhaust Fluid

EEGR-Enhanced Exhaust Gas Recirculation

EPA-Environmental Protection Agency

OMT-Oxygen Transport Membrane

SOFA-Separated Over-Fire Air

α_k – Constant coefficient for the variable temperature

T_p – End point or max temperature for which which a specific product will be completely vaporized.

p- product stream from CDU.

P_{CDU} - Group contain all products of CDU.

Rsd- Residual of bottom fraction from CDU.

EP- End Point Temperature which is the same as Tp.

$V_{CDU,p}$ – Volume flow rate of product stream (p) from CDU.

F_{CDU} – Crude oil feed volume to the CDU.

$X_{CDU,p}$ – Different properties for each product stream (p) leaving CDU.

X_p – The set of all properties for a specific stream (p) leaving CDU.

$T^L_{CDU,p}$ - Lower limit for cut temperature for product (P).

$T_{CDU,p}$ - Cut temperature for product fraction (p) of CDU.

$T^U_{CDU,p}$ - Upper limit for cut temperature of product (p) of CDU.

$Umax_{CDU}$- Maximum feed that can be sent to CDU.

GAMS – General Algebraic Modeling System

A_i – Price of selling product (i) in dollars / barrel.

BP_i - Volume of blending unit (i) in barrel.

B_i - Cost of feed (i) to refinery or CDUin dollars / barrel of crude oil.

F_i – Feed (i) of crude oil to CDU in barrels.

C_i - Operational cost for unit (i) dollar/year.

$D_{i,sw}$ – Cost of switching to fuel (sw) in unit (i)

$Z_{i,sw}$ – Binary variable equal to zero or one, related to use of (sw) fuel in unit (i).

sw – Fuel type used.

y- Technology type used for NOx reduction.

$Y_{i,y}$ – binary variable equal to zero or one, related to the use of (y) technology in unit (i).

$V_{j,p,i}$- Flowrate of product (p) going to unit (i) and coming from unit (j).

$X_{i,F}$ – Property (X) of feed (F) to unit (i).

$X_{j,p}$ – Property (X) of feed (j) for product (p).

$V_{i,p}$ – Volumetric flow rate of unit (i) of product (p).

F_i - Feed flow rate for unit (i).

$V_{i,N}$ – Variable N of unit (i).

$V_{i,p,m}$ – Volumetric flow rate of unit (i) and product (p) to split (m).

$Z_{i,sw}$ – Binary variable of unit (i) for fuel switch to fuel type (sw).

IF – Set of all units in the oil refinery.

$NOx_{i,sw}$ – Amount of NOx produced from unit (i) when switching to fuel (sw).

$E_{i,y}$ – Cost in dollar/Year for using technology (y) with unit (i).

b_x – blending index of property X.

$n_{x,p}$ – index for property X of product (p).

w_p – mass or volume fraction.

$sp.gr_{blended}$ – specific gravity of blended streams.

$RateV_p$ – Volumetric flowrate of product stream (p).

$Sul_{blended}$ – Sulfur content of blended streams.

$RateW_p$ - Mass flow rate of stream (p).

Sul_p – Sulphur content of product stream (p).

N_{RON} - Research octane number.

$N_{RON,p}$ – Research octane number of product stream (p).

RVP – Reid Vapour Pressure.

RVP_{blend} – Reid Vapour Pressure of blended streams.

$(RVPBI)_p$ – blending index for RVP of strem (p) .

CN – Cetane Number.

DI – Diesel Index.

IN_{SP} – Smoke Point Index.

SP – Smoke Point

RateV – Volumetric flow Rate of fuel to viscobreaker.

RateV1- Volumetric flow rate of LN leaving viscobreaker.

RateV2- Volumetric flow rate of HN leaving viscobreaker.

RateV3- Volumetric flow rate of Gas Oil leaving viscobreaker.

RateV4- Volumetric flow rate of Buttom Fraction leaving viscobreaker.

LN –Light Naphtha

HN – Heavy Naphtha

Sul - Sulfur

BBL – British Barrels

SG – Specific Gravity

LNSR- Light Naphtha Straight Run

HNSR- Heavy Naphtha Straight Run

LVGO- Light Vacuum Gas Oil

HVGO- Heavy Vacuum Gas Oil

RON – Research Octane Number

CDU- Crude Distillation Unit

RDHT- Residual Hydrotreater

Visc.- Viscobreaker

GOHT- Gas Oil Hydrotreater

DHT – Diesel Hydrotreater

NHT- Naphtha Hydrotreater

HC – Hydro Cracker

REF - Reformer

References

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Vitae

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2nd Air pollution control:
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