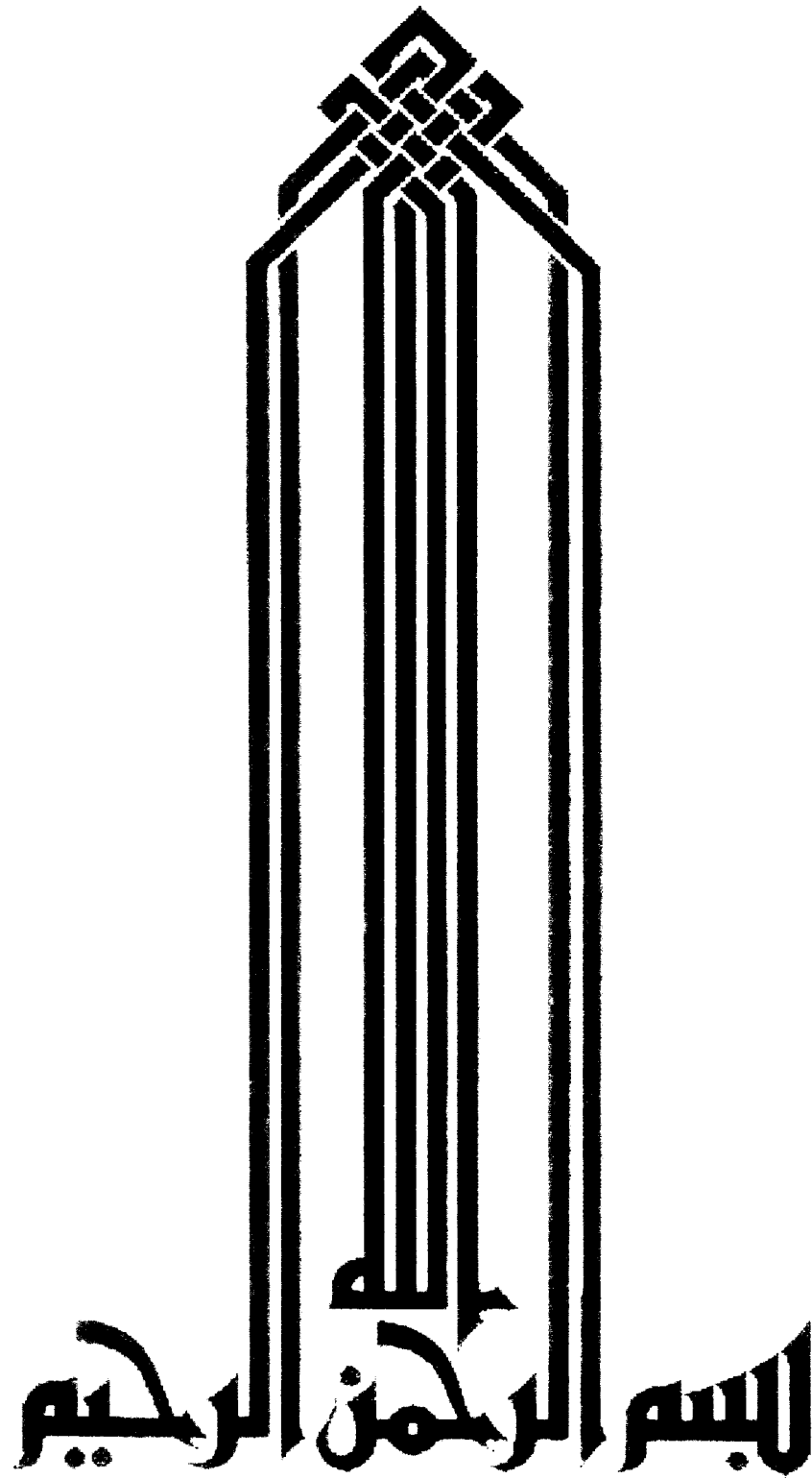


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DISSERTATION

MULTI OBJECTIVE MULTI REFINERY
OPTIMIZATION WITH ENVIRONMENTAL AND
CATASTROPHIC FAILURE EFFECTS
OBJECTIVES

Submitted By

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Department of Chemical Engineering

A dissertation submitted in partial fulfillment of
the requirements for the degree of Doctor of Philosophy

Colorado State University

Fort Collins, Colorado

Summer, 2005

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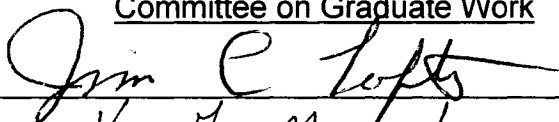
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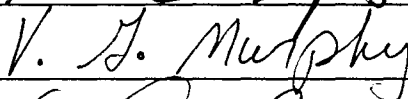
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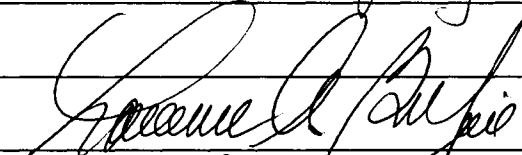
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WE HEREBY RECOMMEND THAT THE DISSERTATION PREPARED UNDER
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MULTI REFINERY OPTIMIZATION WITH ENVIRONMENTAL AND
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PART REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY
IN CHEMICAL ENGINEERING.

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ABSTRACT OF DISSERTATION

MULTI OBJECTIVE MULTI REFINERY OPTIMIZATION WITH ENVIRONMENTAL AND CATASTROPHIC FAILURE EFFECTS OBJECTIVES

Petroleum refining is a capital-intensive business. With stringent environmental regulations on the processing industry and declining refining margins, political instability, increased risk of war and terrorist attacks in which refineries and fuel transportation grids may be targeted, higher pressures are exerted on refiners to optimize performance and find the best combination of feed and processes to produce salable products that meet stricter product specifications, while at the same time meeting refinery supply commitments and of course making profit. This is done through multi objective optimization. For corporate refining companies and at the national level, Intra-Refinery and Inter-Refinery optimization is the second step in optimizing the operation of the whole refining chain as a single system. Most refinery-wide optimization methods do not cover multiple objectives such as minimizing environmental impact, avoiding catastrophic failures, or enhancing product spec upgrade effects.

This work starts by carrying out a refinery-wide, single objective optimization, and then moves to multi objective-single refinery optimization. The last step is multi objective-multi refinery optimization, the objectives of which are analysis of the effects of economic, environmental, product spec, strategic, and catastrophic failure. Simulation runs were carried out using both MATLAB and ASPEN PIMS utilizing nonlinear techniques to solve the optimization problem.

The results addressed the need to debottleneck some refineries or transportation media in order to meet the demand for essential products under partial or total failure scenarios. They also addressed how importing some high spec products can help recover some of the losses and what is needed in order to accomplish this. In addition, the results showed nonlinear relations among local and global objectives for some refineries. The results demonstrate that refineries can have a local multi objective optimum that does not follow the same trends as either global or local single objective optimums. Catastrophic failure effects on refinery operations and on local objectives are more significant than environmental objective effects, and changes in the capacity or the local objectives follow a discrete behavioral pattern, in contrast to environmental objective cases in which the effects are smoother. In addition, crude processing capacity is the main factor affecting the objectives, and results demonstrate the benefit of having more than one crude unit, which gives higher flexibility in running the refinery at low feed rates. Results demonstrate the importance of examining the effects of loss of internal processing flexibility, which may not be clear in either local or global objective functions and can have an effect on products supplies. For all objectives, one refinery price structure creates a conflict with global objectives due to demand constraints imposed on the refinery proper without crediting the refinery's local objective function for these imposed constraints.

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ABBREVIATIONS

Abbreviation	Description
AH, AHVY	Arab heavy crude
AL OR ALT	Arab light crude
API	American Petroleum Institute
ASTM	American Society of Testing and Materials
BPD	Barrels per day
CCR	Continuous Catalyst Regeneration (Type of Catalytic Reforming)
CONST	Constraint
CR	Catalytic Reforming
D	Diesel
DCS	Distributed control system
DHT	Distillate Hydrotreater unit used to reduce diesel sulfur content using hydrotreating process
DMO	Demetalized oil
FCC	Fluidized Catalytic Cracking unit
FO	Fuel oil
HC	Hydrocracker unit
HYSIS	Steady state or dynamic process simulator
IMC	Internal Model Control
JET-A1	Type of jet fuel.

K , KERO	Kerosene
KBPD	Thousand barrels per day
LP	Linear Programming (also known as linear planning)
LSR	Light straight run naphtha
MATLAB	Engineering programming software by Mathworks
MBPD	Million barrels per day
MEROX	MEROX product treatment unit (treats sulfur in refinery Products)
MILP	Mixed Integer Linear Programming
MPC	Model Predictive Control
MVC	Multi Variable Control
N	Naphtha
NLP	Nonlinear Programming
NPA or N+A	Platformer feed naphtha composition of Naphthenes (N) + Aromatics (A)
PIMS (or ASPEN PIMS)	Process Industry Modeling System by Aspen-Tech
PIONA or PONA	Chemical composition of the hydrocarbon stream stands for: Paraffins, Iso-Paraffins, Naphthenes, and Aromatics.
PSA	Pressure Swing Adsorption Unit (produces high purity hydrogen)
Psi	Pressure unit, pound per square inch
Psia	Pressure unit, pound per square inch absolute

Psig	Pressure unit, pound per square inch gauge
R, RC	Reduced crude, also called residue
RFG	Reformulated gasoline
RON	Research Octane Number
RVP	Reid Vapor Pressure, PSIA
SLP	Sequential or Successive Linear Programming
VGO	Vacuum Gas Oil

I INTRODUCTION AND LITERATURE REVIEW

I.1. BACKGROUND

Petroleum is one of the most important sources of power today. In addition, it is the only source of many petroleum-based chemicals known as petrochemicals, which are the basic component of many industries today. The worldwide oil reserve in 1999 was about one trillion barrels. At the production level of 1998, this current oil reserve can be sustained for about 39 years.

Before petroleum can be utilized, it must be fractionated into different cuts. These cuts or products differ depending on the oil characteristics and market demand. Oil is heated and partially vaporized and then is fractionated into several cuts. These cuts are then sent to downstream units for treating or further processing. The process scheme and product use of a typical refinery is shown in Figure I-1, while a detailed refinery flow sheet is given in Figure I-2.

Due to the high market demand for light products and low market demand for heavy fuels, the light cuts of oil from fractionation alone are not sufficient to meet the market demand. The cracking of heavy oils into lighter ones is one solution to this problem.

The first real petroleum refinery was built at Titusville, PA, at a cost of about \$15,000 [25]. In 1998, the total worldwide crude oil production was about

73 million barrels per day. The worldwide refining capacity was then about 67 million barrels per day.

Petroleum refining has developed from simple separation in the early stages to a very complex process today. Early refineries consisted of continuous distillation, vacuum distillation, thermal cracking, and product blending, etc.

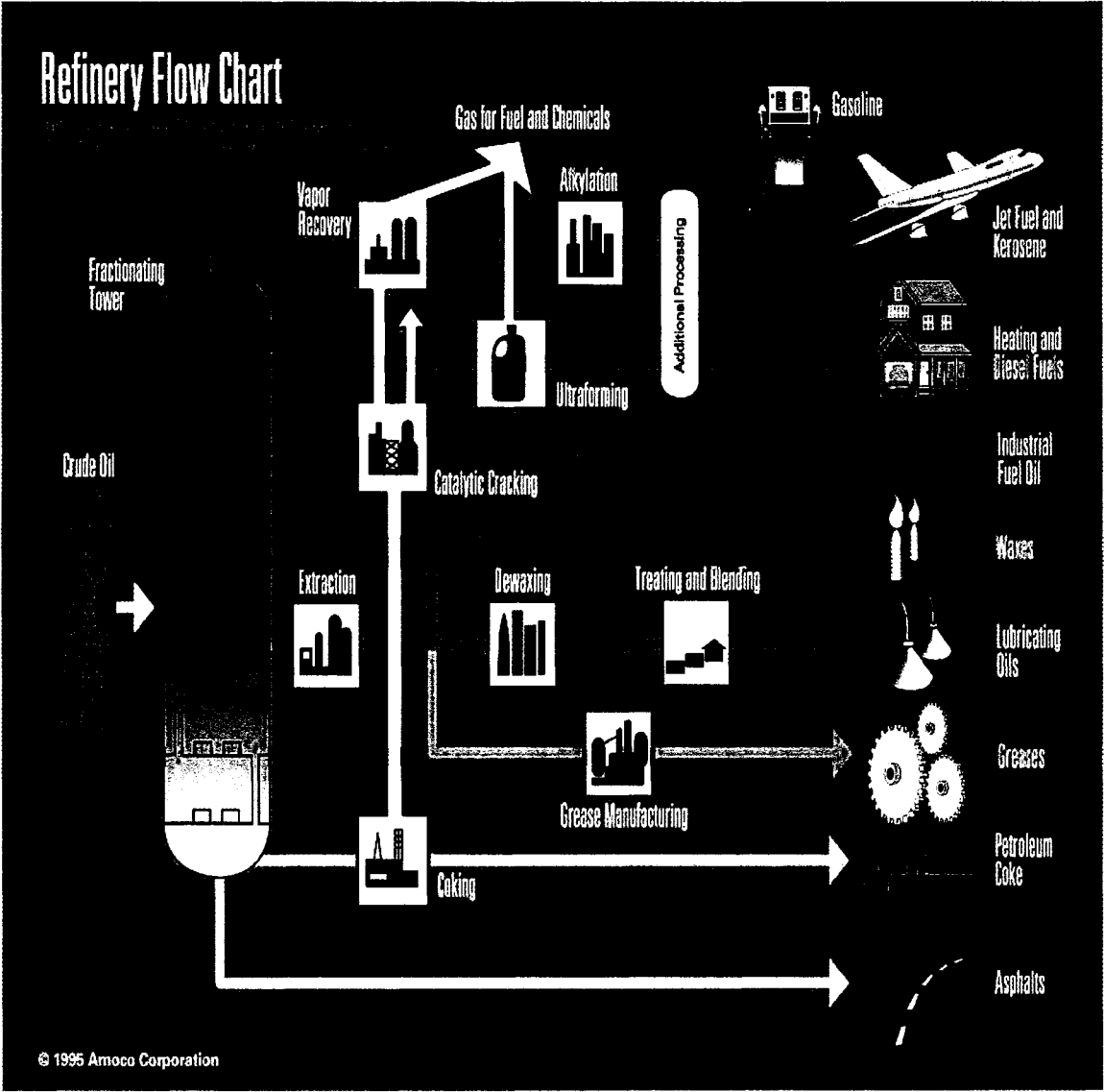


Figure I-1: Refinery Flow Chart, Amoco [16, 20]

Due to the huge demand for aviation gasoline during World War II, the refining industry was obliged to meet this demand both by capacity increase and new technology development. Since that time, many new high efficiency processes have been developed. These new processes include Fluidized Catalytic Cracking (FCC), catalytic reforming, Alkylation, catalytic Desulphurization, Delayed coking, etc.

For decades, the U.S. transportation fuel market has dominated the global petroleum supply. Among all the products made from crude oil, transportation fuels including gasoline, jet fuel, and diesel are produced in the greatest quantities. Passenger vehicles are the largest fuel consumers since most passenger vehicles are fueled by gasoline in conventional combustion engines. These vehicles consume about 8.5 million barrel per day of gasoline, or 12% of the global petroleum demand [25].

Most of the transportation fuel consumed in the U.S. is produced domestically. Due to such massive production, many refineries in the U.S. are fuel-oriented refineries whose main function is to produce transportation fuel. In Europe, where trains, subways, and diesel fueled passenger cars are the most common means of transportation, most refineries are fuel oriented but have diesels as their major products. There are other types of refineries that are oriented for other purposes, as will be discussed later.

I.1.1. Changes in the Refining Industry and Need for Solutions

The refining industry has suffered considerably during the past two decades, so much so that refining is not an economically attractive business anymore. The last US grass roots refinery was built during early 1980s [33]. This is due to increasingly low refining margins and strict environmental regulations.

In reality, many small refineries were forced to quit business since they were repeatedly earning negative net margins, and upgrading small, old refineries is usually economically unfeasible. In the past 8 years, the US refining industry has decreased by 40 refineries, that is, from 192 to 152 [13]. In particular, smaller refineries with zero conversion have closed. Crude capacity has grown by 8% and conversion capacity has grown by 5%. Although 5% seems small, it represents a significant addition of 460 KBPD of new conversion capacity.

In such tight situations, refineries are able to survive and make a return on investment by

1. Being a large, throughput refinery, usually > 300 KBPD.
2. Having a high complexity factor, i.e., being a deep conversion refinery with units that can convert low quality, low price hydrocarbons to high quality, high price products such as gasoline and petrochemical feed stock. Typical units are FCC, Hydrocracker and CCR.
3. Being linked to a petrochemical complex. This is usually possible if the refinery throughput is greater than 200 KBPD. When less than this value, the output of final products is very small and not economically attractive.
4. Having a flexible feedstock processing capability and product diversity

which allows the refinery to shift from one product to another according to demand. This is usually evident and is known in the refining business as summer and winter modes or gasoline versus diesel mode. Some sophisticated refineries have fuels versus petrochemical modes [37]. The demand can change very rapidly and unpredictably. A fire in a Middle Eastern refinery can cause the petrochemical feed stock process to increase in East Asia [33].

5. Having a sophisticated process control systems [19]. In the late 60s and 70s, most refineries were built with pneumatic control systems and analog control. The innovation of the digital computers paved the way for the utilization of new technologies such as DCS, IMC, MVC and MPC. These types of more sophisticated control allowed for narrower cuts and more precise blending of fuels, which eliminate having a large giveaway in products, as is the case with simple controls. For example, an oscillation of 3% in diesel production can overload jet fuel Merox units and hence limit the overall refinery throughput by allotting some of the light diesel oil to the Kerosene section, while on the other peak, 3 % of the diesel is degraded and dumped into the reduced crude, which will subsequently have to be recovered in vacuum units or otherwise be degraded from diesel to fuel oil.
6. Having a clear and comprehensive overall optimization strategy. Since this comprises the main subject of this work, it will be covered in detail later.

I.2. REFINERY OPTIMIZATION

The refining business cannot be economically attractive without including the six above-mentioned points. Optimization is probably the widest and most important among all factors for both old and new refineries. Since one of the optimization tools is a successful process control, the literature on the subject frequently discusses process control under optimization. Moreover, we are controlling the plant to optimize its performance, and optimization can include better control algorithms, DCS, IMC, MVC and customized control philosophies for special tasks.

In addition, in a world that is so dynamic and changing politically and economically every day, it is possible to have a number of feed stocks with different properties and specifications such as API gravity, Sulfur %, ASTM distillation, etc. It is here that the art of planning and scheduling of refining feeds and products becomes paramount. A change of a few cents per barrel in the price of a specific feed to a refinery can generate a change of hundreds of thousands of dollars, if not millions, in a refinery's profits. Consequently, a refinery may be forced to process some kind of crude other than the one the refinery was originally designed for. Several crudes charged to the same or different distillation units may also be processed simultaneously. Proper optimization, including an understanding of which crude is better for which product while knowing the capabilities and limitations of all process units and logistics in the refinery, can save millions.

The same can be said about final products, since it is possible for a refinery to import a finished product from another source and use it as a blending component for the refinery's intermediate products. For example, a refinery can import very low sulfur diesel oil to blend with refinery-processed high sulfur oil to turn out a final product that meets a medium sulfur diesel oil specifications.

I.2.1. When Is Optimization Important?

As mentioned earlier, it is best to have a large refinery with deep conversion capabilities integrated to a petrochemical complex. Even in such a case, optimization is so vital that it can save millions of dollars. The main use of optimization in this case is both economic and for the purpose of meeting the environmental regulations and products specs.

Unfortunately, this is not always the case. Most of the world's refineries include different processing units. Most of the refineries in the USA and Europe were built during the period 1940-1970. Many of these refineries consist of small units with many limitations, including:

1. High maintenance cost due to age and old process and equipment technology.
2. High operating cost due to size limitations. The same number of employees is usually required to run a 20 KBPD or a 200 KBPD. However, large processing units are usually newer with better controls and lower labor requirements.
3. In a highly competitive field, it is not usually economically feasible to build

new deep conversion units or a petrochemical complex with such size limitations.

4. Stringent environmental regulations sometimes make it impossible for small refineries to continue operating while simultaneously meeting regulations and making profit.

Consequently, for most small-size refineries, optimization is a matter of life or death. It is therefore no wonder that oil companies are spending millions on optimization studies and packages, as well as on hardware optimization, such as improving energy integration. In the US, many small refineries, especially those belonging to large refining corporations, have had to quit business or sell out to independent refiners who are able to get some breaks on environmental regulations and increase the refining margin by having less corporate overhead costs.

I.2.2. Optimization and Process Control

The common goal of all refiners is to provide safe, profitable, quality product manufacturing. Process control and optimization have become indispensable tools for realizing this goal. Significant advancement in instrumentation and computers has made the implementations of process control and optimization cheaper and more reliable.

Process control is concerned with operating a plant in such a way that the product quality and production rate specifications are met in a safe and reliable manner while meeting all other objectives such as environmental and process constraints.

The basic task for a controller is to maintain a process variable at a given set point. These set points must be as economically favorable as possible. This economic target can be expressed in different forms: maximum production, maximum profit or minimum cost.

Choosing the set points that make the process most profitable while observing process constraints and meeting all product specifications is an optimization problem. In the past, operators and process engineers based on their experience and intuitions on these set points. However, such a decision-making approach cannot be consistent due to the differing backgrounds of the people making the decisions. In modern refineries, a more systematic approach like that given below is followed:

1. A planner/scheduler usually develops an operating plan for the next several days, given current levels of crude stocks, operating capacities, off takes and inventory constraints. This is generally done using Linear Programming (LP).
2. After the solution is found, the planning engineer sends the values in the solution as set points to engineers in unit operations.
3. In plant operation, the engineers in a specific unit then use the information provided to choose the set points for each respective control loop as well as for those that are not provided by Linear Programming.

I.2.3. Refinery Optimization Objectives

Recent works cover many subjects that are elements of the overall refinery optimization scheme. These refer to optimization for better control, scheduling, or better heat integration and hydrogen management. Frequently, optimization is covered under the scope of optimal control strategy.

Heat integration, steam and hydrogen management are beyond the scope of this work. An exception is cases in which the optimization of such items is related to a change in operating conditions or parameters such as flow, operating temperature, type of feed, diverting one or more intermediate products from one unit to another, or in a refinery-wide optimization model (such as utilization of hydrogen from the CCR unit instead of producing fresh hydrogen in the PSA unit).

The first type of heat integration requires hardware management, such as changing the heat exchanger train configuration. The change of the cooling fluid type or waste heat recovery (such as recovering heat from an FCC unit) is usually a design problem requiring mechanical work. However, this is usually expensive and is beyond the scope of regular optimization models which optimize existing hardware for optimum goals, which is what most refiners are seeking.

Zhang et al [41] addressed the problem of simultaneous optimization in integration in overall refinery planning, where they considered the allocation of steam and hydrogen into the overall refinery model. The hydrogen requirements were linked to the liquid flow model. Depending on the fluid properties of the liquid streams, the hydrogen requirements were calculated and included in the model. However, Zhang's work is based on a linearized MINLP in which the

nonlinear functions of the model were linearized using two different linearization techniques.

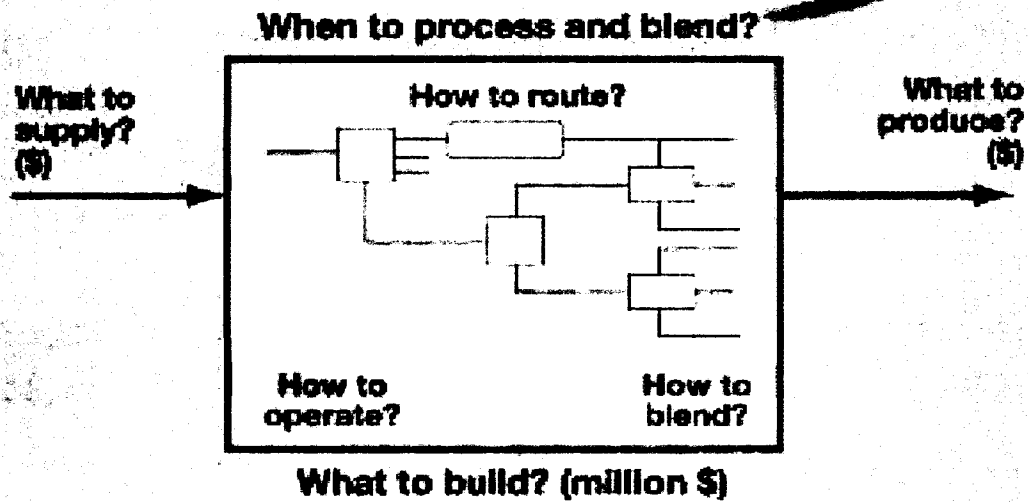
There are other applications of optimization of oil and gas processes that are not necessarily related to refining processes such as methane management from wells [40]. Pinto et al. [31] discussed planning and scheduling applications for refinery operations. Firstly, the development of a nonlinear planning model for refinery production was presented. The model was able to represent a general refinery topology and allowed the implementation of nonlinear process models as well as blending relationships. The second part of their work addresses oil refinery scheduling problems that were formulated as mixed integer optimization models and relied on both continuous and discrete time representations.

1.2.4. Refinery Optimization with Linear Programming

Dantiz introduced Linear Programming (LP) in 1947 [27]. In LP, all the constraints and objective functions are linear. One of first principal uses of LP was to solve refinery optimization problems. In 1956, Symons used LP to solve a simplified gasoline-blending problem. Since then, LP has found wide acceptance in the refining industry.

LP is a major planning and scheduling tool due to its ease of use and faster convergence. A common method for solving LP optimization problem is the use of the Simplex method that was introduced by Dansig in 1947 [10, 24, 27]. The problem with using LP in modeling refinery processes is that the nature of the refining processes is mainly nonlinear. To understand the difference, we

have to distinguish between refinery process modeling and production planning and scheduling. Hartman [17] described the difference and usage of each and interactions between models, as is shown in Figure I-3 and Figure I-4.



<u>Decisions on</u>	<u>Model for</u>	<u>Objective</u>
What?	Planning	Integrated economics
How?	Operation	Detailed economics <ul style="list-style-type: none"> • Plant optimization • Blend trimming
When?	Scheduling	Check on feasibility <ul style="list-style-type: none"> • Time (arrival/liftings) • Volume (empty/full)

Figure I-3: Decisions and Models [17]

In planning and scheduling, the constraints are linear (supply and demand). The objective function is also linear, and if not it can be linearized with acceptable accuracy for simple supply chain problems [38]. On the other hand, for refining industry process modeling, the relations describing the conversion

and treatment processes are nonlinear by nature. Other variables, such as reformer platinum catalyst activity, temperature, feed quality, PIONA, and product properties such as RVP and RON, are highly nonlinear and cannot be assumed to be linear for a broad range of operating parameters [41]. Even in the final product blending, such as gasoline blending, the blending process can originate from non-ideal mixing processes and lead to non-linearity in the blending curves [33].

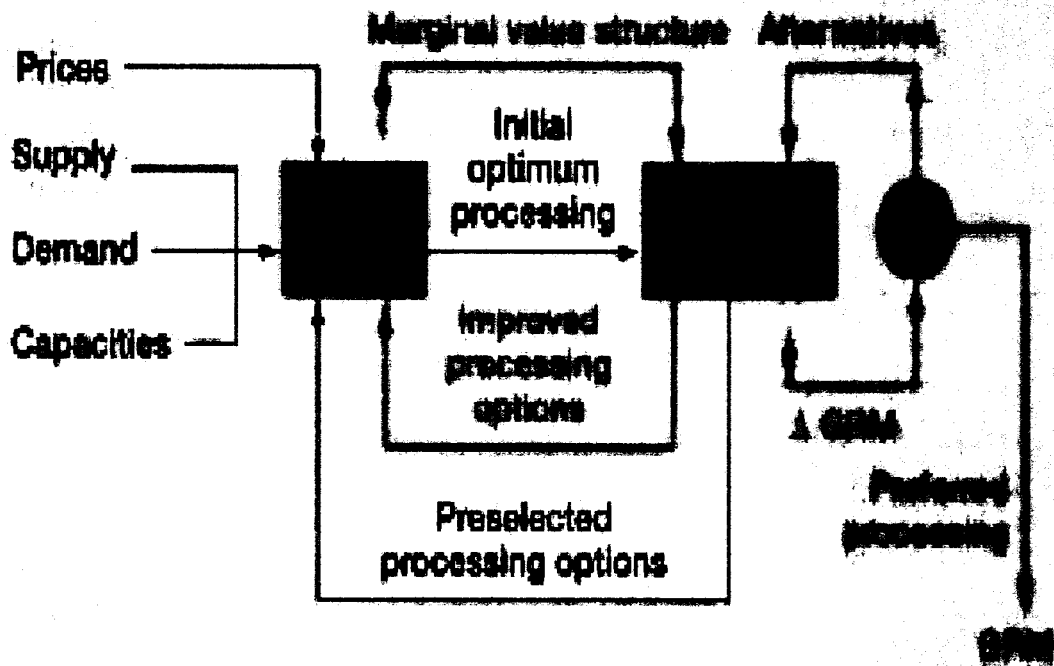


Figure I-4: Interactions between LP model, simulation model and user [17]

Plant optimizers are planning models that cover a smaller domain than the refinery-wide planning model [17]. Such models are intended to determine plant

operating variables (such as cut points and severities) that maximize the (dollar) added value obtained from each individual processing unit.

I.2.5. Single-Unit Versus Multiple Unit Optimization

Single-unit optimization needs correct price information concerning the intermediate streams, which is not always available. Intermediate product price is a function of quality and product rate. To solve this problem, some engineers used the shadow prices of the refinery LP to evaluate the prices of intermediate products. A shadow price is the change in the optimal value of the objective function per unit change in an active constraint. However, the shadow prices of LP are not valid when the operations shift to different product qualities or a different schedule. Single-unit optimization based on imprecise price information can result in conflicts with plant-wide operation strategies.

In order to overcome the inherent disadvantages of LP and single-unit nonlinear optimization, Li [25] developed a new approach for tackling the optimization problem in the refinery. In his work, several nonlinear single-unit models are integrated into a refinery-wide model, which is used in nonlinear optimization to determine the optimal operating conditions for the entire refinery. He did this using the following procedure:

1. Developed nonlinear single-unit models for the important processes in a refinery.
2. Integrated developed single-unit models into an overall refinery model.

3. Carried out nonlinear optimization using the developed models to determine the optimal operating conditions for the entire refinery.
4. Evaluated the incremental profit of using such an optimization approach by-comparing it with results from normal operating conditions.
5. Compared refinery-wide nonlinear optimization with single-unit nonlinear optimization.

1.2.6. Environmental Optimization

Significant work has been done on the environmental optimization of process industries, but no major work is reported specifically on refineries. Most of the work on optimization relates to the design phase, such as designing new plants for better compliance with increasingly stringent environmental regulations. Fu [15] studied the multi objective optimization of chemical plants with environmental considerations. His main contribution was the inclusion of the multi objective algorithm in the commercial software ASPEN. Shelly [34] focused on environmental optimization from other points of view, including product allocation and optimization of hydrocarbon resources, such as converting hydrocarbon waste into value-added products.

Environmental regulations can affect the overall supply/demand chain and the allocation of feeds and products. For example, it may be more desirable to operate an HF Alkylation unit that is in a remotely located refinery than operating the same unit in an urban refinery.

One of most relevant works in this field was done by Al-Sharrah, et al. [1, 2]. In their work, a model with an environmental objective is presented. The system is formulated as a mixed-integer linear programming model in which new value-added products are produced from basic feedstock chemicals. The optimal set of processes is selected with the objective function of sustainability. Sustainability is quantified by a health index of the chemicals and increasing profit represented by process-added value. The model is applied to the case study of planning the development of the Kuwaiti petrochemical industry.

I.2.7. Catastrophic Failure and Strategic Objective Optimization

With the increased risk of war and terrorist attacks, refineries and fuel transportation grids are targets of possible catastrophic events since they supply the fuels to essential nodes such as power plants. However, not much attention has been paid to this area until recently. Most of the literature has concentrated on the effects of process accidents on refinery emissions and safety.

For some refiners, the optimization scope might be instability and phase equilibria research rather than economic considerations [8]. In such a case, the primary goal is to determine the optimal stable operating conditions for a complex process rather than the best operating conditions for increasing the economic or environmental objective functions. This is particularly important in processes in which the safety or stability of a reactor system is a major concern, as it is in old units in urban areas or units that have mechanical limitations. Operators tend to operate these units at the most stable conditions or at lower reactor temperatures

to avoid runaway temperatures, which may not constitute optimal operating conditions from an economic point of view.

Khogeer [23] observed that a fluid catalytic cracker FCC reactor that had a hot spot due to coke build up might cause a bulge in the reactor dome. The main concern before the shutdown was to operate the unit under safe and stable conditions that could keep the unit running at even lower severity and lower gasoline RON until the next shutdown.

1.2.8. Process Modeling

Not much work has been reported in the literature concerning modeling all refinery processing and blending units. Instead, most of the published research has focused on the tray-to-tray rigorous modeling of atmospheric and vacuum towers.

Probably one of the most complete models for refinery-wide optimization is the work of Li [25], in which he constructed a refinery model to be implemented for refinery-wide optimization. He mentions that a dynamic model using an "open-equation" approach for the control study of a crude unit uses 34 pseudo-components to represent the crude feed and has 2297 differential/algebraic equations, 263 fixed external variables, 9 external manipulated variables, and 2297 dependent variables [25].

I.2.9. Petrochemical Integration

In the past 10 years, the return on replacement capital in the U.S. petrochemical industry has averaged 15.6%, and that of refining has averaged 2.4% [3]. Anon [3] illustrated the benefits of integrating existing refinery operations into petrochemical production. These benefits are:

1. Reduced capital investment or working capital due to efficient infrastructure utilization.
2. Reduced fixed costs as a result of shared services
3. Optimization of overall refinery product yields.
4. Higher value of transfer streams and products.
5. Petrochemical downturns tempered by more stable refining cycles.

Table I-1 shows refinery streams that provide feedstock for a petrochemical plant. Fluid catalytic cracking units (FCC) provide ethylene, propylene, and butylenes. These products can also be produced from delayed cokers but in smaller quantities. Catalytic reformers produce aromatics, such as benzene, toluene and mixed Xylenes known in industry as BTX.

A typical aromatics complex produces benzene and paraxylenes usually from straight run naphtha which is in the range of C₅-C₉. It consists of a BTX separation and extraction plant, as well as a mixed Xylenes separation and Isomerization plant. Toluene and C₉⁺ aromatics, byproducts of the aromatics extraction facility, are used as high-octane gasoline blend stock. Raffinate, also a byproduct, is used for the refinery light-naphtha product. Returns on incremental

investment to achieve integration are significantly higher, 28% on average[3].

The low refinery margins can be offset by the stronger petrochemicals returns.

Table I-1: Petrochemicals from Refinery Streams [3]

Refinery stream	Petrochemical stream	Alternative refinery use
FCC off gas	Ethylene	Fuel gas
Refinery propylene (FCC product)	Propylene	Alkylation/polygasoline
Reformate	Benzene, toluene, Xylenes	Gasoline blending
Naphtha and LPG	Ethylene	Fuel gas
Dilute ethylene (FCC and delayed Coker off gases)	Ethyl benzene	Fuel gas
Refinery propylene (FCC product)	Polypropylene, Cumene, Isopropanol, Oligomers	Alkylation
Butylenes (FCC and delayed Coker)	MEK (Methyl Ethyl Ketone)	Alkylation, MTBE
Butylenes (FCC and delayed Coker)	MTBE	Alkylation, MTBE
Refinery benzene and hydrogen	Cyclohexane	Gasoline blending
Reformate	Orthoxylene	Gasoline blending
Reformate	Paraxylene	Gasoline blending
Kerosene	n-Paraffins	Refinery product
FCC light cycle oil	Naphthalene	Diesel blend stock

As mentioned before, Al-Sharrah, et al. [1, 2] covered the subject of planning a petrochemical industry with environmental considerations; the main indicator used was sustainability using the health index. Redwan, et al. [32] illustrated the benefits of using light naphtha as a petrochemical feedstock in Saudi Arabia. Light naphtha is not a valuable product and is usually exported to countries that have naphtha cracking facilities to be utilized for various petrochemical uses.

II SCOPE OF WORK

II.1. DISSERTATION TOPIC

The topic of this dissertation is "Multi Objective Multi Refinery Optimization with Environmental and Catastrophic Failure Effects Objectives." The problem of optimizing a chain of refining and demand nodes is addressed, including case studies of several refineries, demand points, various crudes, etc. Multi objective includes environmental and safety concerns. Emphasis was placed on the use of commercial software whenever possible.

II.2. SPECIFIC GOALS

This work was begun by constructing a global optimization model and comparing the results from this model to the results of a single refinery optimization model. This is important in a market that changes daily, with different supply, demand, and process conditions. This work includes a consideration of optimizing different feeds and products available to various kinds of consumers at different prices. It also calls for better resource allocation.

The model was then extended to cover multi objective intra optimization, addressing essential constraints such as environmental regulations and their ef-

fect on the overall supply/demand chain and the allocation of feeds and products depending on these regulations.

As one of the major goals, emphasis was given to the use of commercial software whenever possible so that the package was user-friendly to people in the industry and could be integrated into the existing software that refinery engineers are familiar with, such as PIMS, HYSIS, ASPEN product, etc.

II.3. DISSERTATION CONTRIBUTION

The contribution of this dissertation to the field of chemical engineering in general and to the fields of petroleum refining and refinery optimization in particular is intended to be as follows:

1. It covers the area of refinery-wide optimization in particular, which is rarely covered in literature. Most of the work done has been either on optimization using advanced process controls or optimization on single units.
2. It emphasizes the concept of multi objective intra-refinery optimization. This is topic of importance in deciding where to build new plants or how to better utilize a facility that is more bound by environmental constraints than others. For example, a refinery in an urban location that is constrained by emissions regulations can create more profit by shutting down a high emissions unit such as a Coker unit and utilizing the remainder of the plant by expanding the greater profit-making facilities having less environmental impact, such as CCR or Isomerization units. A product that

cannot be produced except from emissions-extensive units can then be produced at some remote area refineries with less stringent environmental constraints. A real world example is that some refiners are thinking of shutting down HF Alkylation units in the Los Angeles area and building or expanding the same unit in Nevada which has less environmental stresses than California.

3. This work introduces the concept of optimization through operating a refinery or chain of refineries in order to produce a typical high profit refinery product such as fuel or asphalt, or sacrificing fuel production in favor of producing petrochemical feedstock for downstream petrochemical complexes, which can result in increasing the overall profit for the refining corporation even though it may reduce a single refinery's profit margin.
4. It covers the advantages of integrating the three main oil industry's decision-making tools, which are:
 - a. Linear planning software used for feed and product allocation, as well as planning and scheduling for maximum profit.
 - b. Simulation software used to predict optimum operating conditions for meeting product specs and quantities set by the LP.
 - c. A plant optimization tool that optimizes the operation of the whole network to obtain maximum benefits, given constraints related to process, capacity, environment, and any additional constraints.

5. It identifies the operation of a refinery or a supply/demand chain consisting of multi refinery, multi feed and multi demand hubs under catastrophic failures resulting from potential terrorist attacks, wars, or natural disasters. This is in particularly important since oil is the main source for most of the world's power and desalination plants, thereby making it a potential target.
6. It utilizes commercial user-friendly engineering packages whenever possible. This is extremely important if this work is to be of use to the refining industry, since most of the literature is academically oriented and written as a black box, which renders it incapable of upgrading. In addition, refining engineers do not have confidence in using the results of academic research for actual plant operation since they either cannot edit and debug the program, or do not have programming skills in the languages in which the program was written.

III MODEL FORMULATION

III.1. FACTORS AFFECTING MODELING

The following are key considerations when developing a realistic refining model:

1. The mathematical statement of the problem should be as simple as possible.
2. The variables to be selected for manipulation should have significant effects on the objective function.
3. The number of constraints and variables should be kept to a minimum without losing sight of the goal in order to obtain the desired results in the least possible time.
4. Proper scaling should be done so that all terms in the objective function are of the same order of magnitude.

III.2. ASSUMPTIONS

In order to simplify the problem, the following assumptions were made:

1. Steady state operations with no holdup time, no accumulation, and the changeover time of blends has been neglected. Changeover time is the time needed to switch from one product to another in a tank.
2. Perfect mixing occurs in blending tanks.
3. Only specific key components in crude or blended oil fix the property of crude and blended oil.

These assumptions are realistic for the purpose of this work since the objective is the overall optimization of the system where dynamic factors such as accumulations and holdup times do not have significant effect and do not appear in the objective function.

III.3. PROCESS DESCRIPTION

In this research, we were not interested in detailed tray-to-tray simulation. Instead, we concentrated on economic optimization of an entire refinery. This optimization can be carried out in a multi refinery approach, while taking each individual refinery as a subsystem. Thus, optimizing each refinery would optimize the whole grid. For a more global picture, the model should carry out optimization of all the units in the network and determine the global optimum, even if it is not an optimum for a single refinery. In order to extend a model formulated for a single refinery optimization to include multi unit multi refinery, the following two factors should be considered:

1. Correct cost of intermediate product transfers between refineries.

2. Adequate indexing of the process units and refineries in the model. For example, we can have FCC_j where j refers to the jth refinery.

III.4. REFINERY UNITS MODELING

To simulate a refinery in an LP optimizer program, the refinery data must to be obtained in one of following ways:

1. A model should be constructed for all refinery units, as well as product blending. This can be done by MATLAB using basic equations, or it can be carried out more efficiently on any simulation package, such as HYSIS or ASPEN PLUS.
2. Real plant data obtained from test runs. Usually these test runs are carried out at different severities and operating conditions to be able to correlate the refinery units' capabilities at each different point for different products and feeds schemes.

For this work, it was decided to use real data from existing refineries to make the data more accurate. Usually these data are entered into the LP program as a delta-base method, which permits the program to correctly predict the products' slates and physical properties at each point.

III.5. CREATING THE SUPPLY/DEMAND CHAIN

A Supply/Demand chain (S&D) was constructed that included the major refinery feed, processing, storage, and consumptions nodes. An S&D chain is required for good resource allocation and on-time product supplies. To have a good model of a refining system S&D chain, the following should be identified:

- a. Different crude types.
- b. Different feeds other than crude, including fuels (condensate, fuel gas, reduced crude, MTBE, etc.).
- c. Different refineries, with each refinery having different process units.
- d. Process limitations and capacities. For example, CCR maximum reactor temperature in refinery A is 500C. Feed capacity at this reactor temperature cannot exceed 7 KBPD.
- e. Different transportation media such as tankers, pipelines, and trucks.
- f. Major consumer nodes, such as desalination plants, power plants, etc.
- g. Markets and product requirements for that market, such as gasoline, diesel, fuel oil, etc., for both summer and winter modes.
- h. Supply/demand growth per year.

At a later stage, the model was modified to incorporate Multi Nodes and Multi Objective Optimization. Figure III-1 below shows a schematic example of a simplified supply/demand chain that gives an example of feed pools available to refineries, refineries as blocks, internal units in refineries, major consumption nodes, and interconnections between the refineries and within the chain.

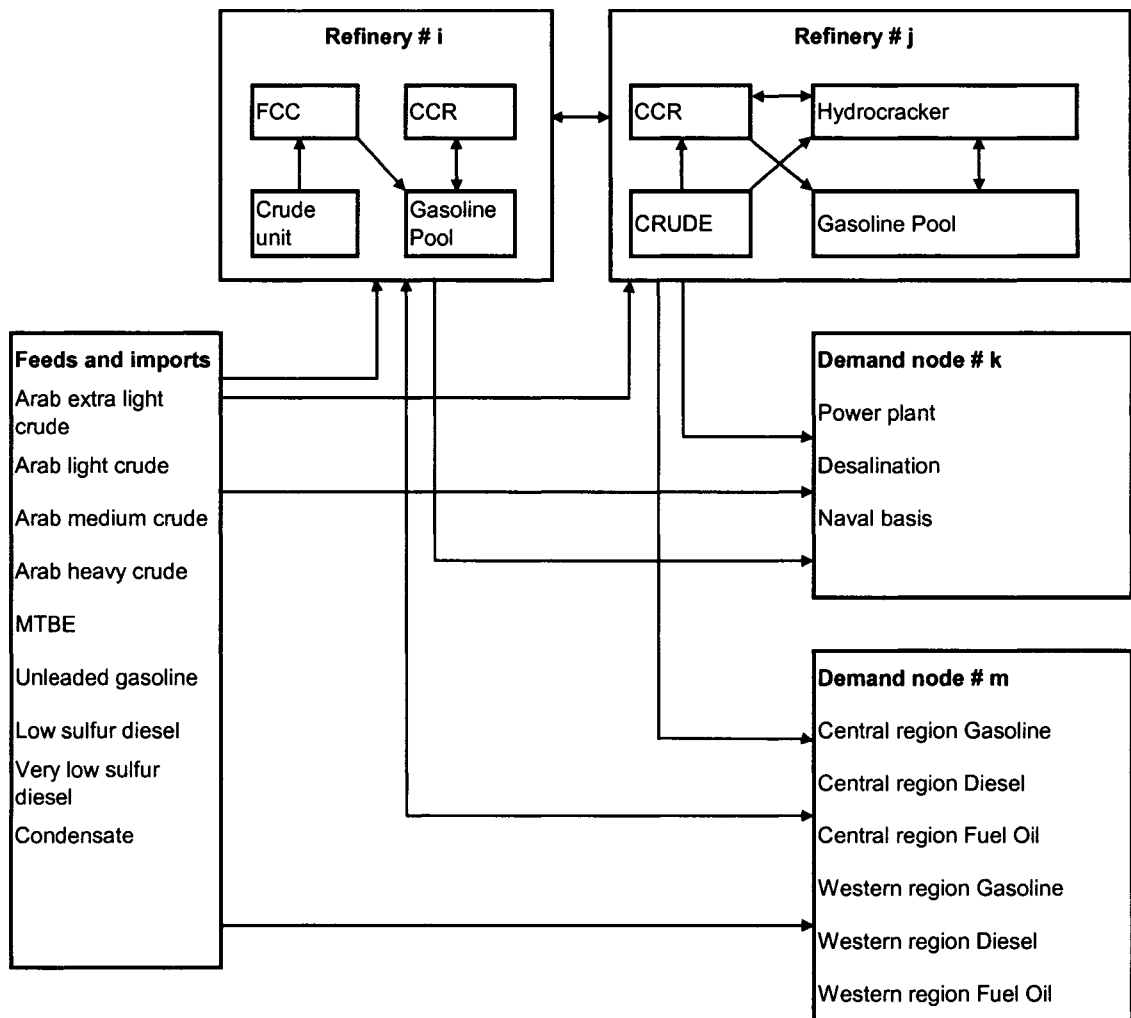


Figure III-1: Refining Supply/Demand Chain

III.6. ENVIRONMENTAL OBJECTIVE MODELING

To properly model environmental objective effects, it is necessary to define the environmental constraints and divide them into different groups depending on their effect on the refining operations. For this work, the environmental constraints were categorized into tolerable and intolerable.

Tolerable constraints apply to environmentally polluting substances or emissions that are harmful to the environment; however, despite their adverse effects such substances can still be released into the environment, but only within certain limits. For example, a refinery can flare off-gases despite the toxic emissions produced. However, penalties should be imposed on tiers to simulate the cost of damages to the environment. Another example of tolerable constraints is to build an HF Alkylation unit in an urban location refinery, even though adhering to environmental guidelines will be more expensive.

Intolerable constraints apply to the category of emissions and environmentally hazardous materials that may not be released, or exceed a certain specified limit. For example, depending on the country and location, H₂S emissions cannot exceed 10 PPM, and Hydrofluoric acid cannot be released into atmosphere under any circumstances.

The procedure of writing the environmental effects as constraints in the model was as follows:

1. First, major and easily implementable environmental constraints were defined. This might include maximum NO_x from FCC and off-gas flaring. Other limitations such as maximum sulfur content in diesel may not be directly related but are rather a product specification.
2. These critical nodes were then specified and the limit for each node was found.
3. These limits were noted down as environmental constraints.

4. The intolerable environmental constraints were linked to oil flow. These data were mostly taken as output from a process simulator or actual plant data and plugged into the LP software. For example, in order to produce NO_x less than 10 PPM, FCC feed from crude unit # 1 should be less than or equal to 3 KBPD at a reactor temperature of 530° C. This is a function of the crude assay and the specific process conditions for each unit.
5. For tolerable environmental constraints, weights were constructed to compensate for the more hazardous wastes. For example, Product A cost 10 \$/BBL from 100-1,000 barrels and it costs one dollar more for more than 1,000 barrels. Thus the cost per barrel will increase as the volume increases. These weights were linked to the constraints and generated a final set of constraints for tolerable hazardous waste to be included in the model, as can be seen in Figure III-2 for a very simplified model.

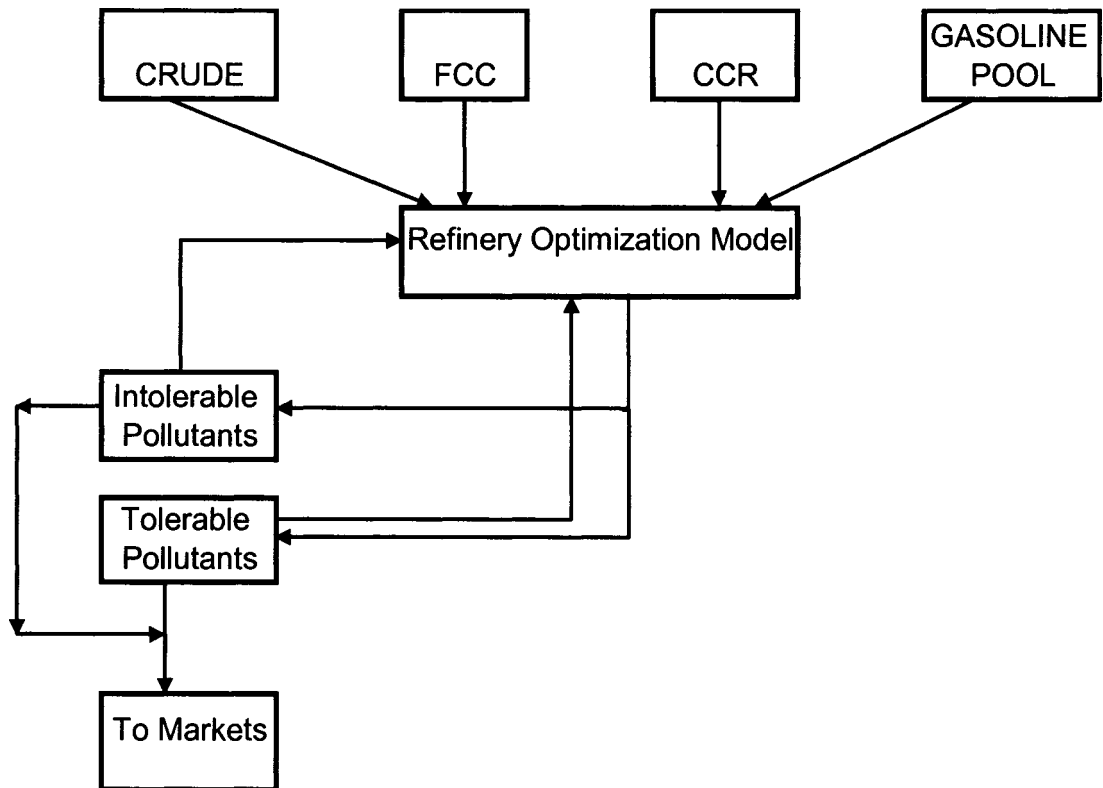


Figure III-2: An Example of an Environmental Objective Formulation into Tolerable and Intolerable Constraints

III.7. CATASTROPHIC FAILURE OBJECTIVE MODELING

The idea behind having an optimization scheme to cover catastrophic failure is to study the effects and explore alternatives of refinery operations and product supply to markets when a catastrophic failure resulting from a process accident or deliberate act such as terrorism causes partial or total failure of the system. This type of condition should be divided into two groups:

- a) Catastrophic failure having on or off (0/1) operations. 0/1 indicates that a particular piece of equipment or process unit is either working or not. For example, in the case of pipeline rupture, the pipeline usually cannot be used and should be shut down. For this group, constraints were treated as binary (0/1) constraints in the model.
- b) Relative increased risk of operations due to process or non process reasons. This includes the risk of war and increasingly the risk of terrorist acts such as the hijacking of tankers or trucks. For example, in case of war in the Arabian Gulf which had been historically a hot zone, tankers are penalized \$1.0 per barrel for shipment from the Arabian Gulf but not from the west coast of the Arabian Peninsula on the red sea since tankers will have less risk.

III.8. OBJECTIVE FUNCTION

The objective functions for refinery-wide or multi refinery optimization vary and depend on the objective in place and the weighting of each variable. Usually all optimization models will include maximum profitability as the main objective, given the crude slate and refining facilities. In the objective function, only the feed cost, operating cost, and revenue from product sales are taken into account. Fixed costs, such as salaries, are excluded from the objective function, since they are not variables and will not change upon optimization.

The operating cost includes catalyst, additives, fuel, power, and cooling water. These costs are combined into one category called utility. Since the operating costs are much smaller in comparison to other items in the objective function, this simplification has no significant effect on the optimization results.

When catastrophic or environmental objectives are included, the two objectives may be in conflict. There is no way to simultaneously maximize total profit and minimize environmental impact, but a trade-off exists.

The objective function can be expressed mathematically as follows [6]:

$$\text{Maximize } \Phi = P_1 - P_2 - P_3 - P_4, \quad \text{III-1}$$

or in more standard form:

$$\text{Minimize } \Phi = - (P_1 - P_2 - P_3 - P_4), \quad \text{III-2}$$

where

- Φ is the profit-based objective function,
- P_1 is the selling price of the products, which constitutes the major income of a refinery,
- P_2 is the price of the raw materials,
- P_3 is the operating cost,
- P_4 is the product-property related parameter and is usually set to zero.

P_1 is given by the following equation:

$$P_1 = \sum (\text{Prod}_j \cdot \text{Price}_j), \quad \text{III-3}$$

where

- $j = 1, \dots, 7$ is the product for the refinery, such as LPG, gasoline, etc.,
- $Prod_j$ is the production rate of product j , (BBL/Day),
- $Price_j$ is the price of a unit quantity of product j , \$/BBL.

P_2 is given by the following equation:

$$P_2 = \sum (Feed_k \cdot Price_k), \quad \text{III-4}$$

where

- F is the feed or imported stream flow rate (BBL/Day). This can be crude oil, an intermediate product (such as vacuum gas oil VGO for FCC feed), or a finished product (such as ultra low sulfur diesel) imported from other sources,
- $Price_k$ is the cost of the feed, \$/BBL,

P_3 is given by the following equation:

$$P_3 = \sum (utility_n \cdot UC), \quad \text{III-5}$$

where

- $Utility_n$, (m^3 /Day) is the utility consumed in process unit n ,
- UC is the cost of the utility (\$ / m^3).

III.9. CONSTRAINTS

Refinery constraints are usually capacity limits, process variable constraints and product specifications. Other constraints such as environmental constraints can be added as limit or penalty constraints. Table III-1 gives an example of constraints for a typical mid-size, medium-complexity refinery.

A capacity limit is the maximum throughput of a unit obtained from the design or test runs. Process variable constraints represent the maximum or minimum value of a process variable. If the value of a process variable is outside the interval defined by its maximum and minimum values, violation of safety regulations or damage to the facility may occur. For instance, temperature cannot exceed the metallurgical design limit of the contacting materials.

Product specifications are constraints on the final or intermediate products, and they are different for each product. In addition, each product can have different grades. For example, several products are obtained from a crude unit such as Naphtha (N), Kerosene (K), Diesel (D), and the Residue (R). Each of these products is characterized by one or more properties such as Reid Vapor Pressure (RVP) for Naphtha, flash point for Naphtha, Kerosene, and Diesel; end point for the Kerosene; and recovery at 366° C for Reduced Crude (RC).

However, product-property constraints are normally not used in the optimization of petroleum refining since on-line sensors needed for measuring these properties are expensive and difficult to maintain and, hence, seldom used. Moreover, no equations exist with acceptable accuracy in relating measured operating variables to product properties to be used in the optimization.

Table III-1: Typical Refinery Constraints [37]

	Unit	Constraint Name	Lower limit	Upper limit
Capacity constraints	CDU	Throughput, KBPD	40	100
		Naphtha, %	18	26
		Kerosene, %	10	25
		Diesel, %	20	40
		Residue, %	37	NA
	FCC	Throughput, KBPD	15	25
		Gasoline, %	40	60
	CCR	Throughput, KBPD	15	25
		Gasoline, %	65	82
	H/C	Throughput, KBPD	20	25
Process constraints	CDU	Heater outlet temp, C	NA	370
	FCC	Max reactor temperature, C	NA	530
		Regenerator max temp, C	NA	760
	CCR	Max reactor temperature, C	480	514
	H/C	Max reactor temperature, C	480	600
Product constraints	Gasoline	RVP, Psia	7	11
		RON	92	95
	Kerosene	Flash Point, C	38	--

These constraints can be written as:

$$CH = \sum (\text{Feed}_k \times \text{wt}_f)$$

$$N \geq 0.18 \text{ CH}$$

$$N \leq 0.26 \text{ CH}$$

$$K \geq 0.10 \text{ CH}$$

$$K \leq 0.25 \text{ CH}$$

$$D \geq 0.20 \text{ CH}$$

$$D \leq 0.40 \text{ CH}$$

$$RC \geq 0.37 \text{ CH}$$

$$\text{Crude charge} \leq 100$$

$$\text{Crude charge} \geq 40$$

$$\text{FCC charge} \leq 25$$

$$\text{FCC charge} \geq 15, \text{ etc...}$$

III.10. TERMINATION CRITERION

The termination criterion is

$$| \Phi_{n+1} - \Phi_n | < \epsilon, \quad \text{III-6}$$

where Φ denotes the value of the objective function and the subscript indicates the iteration number. ϵ represents the absolute difference in magnitude of the objective function in two successive iterations; this is a user-given value. For the recursion part, which will be discussed later, there are two recursion tolerance options [30]:

- Absolute Error Tolerance $ATOL = | (P_c - P_p) |$, III-7

- Relative Error Tolerance $RTOL = | (P_c - P_p) | / P_p$, III-8

where

P_c = Current Property Value,

P_p = Previous Property Value.

III.11. DECISION VARIABLES

Decision variables are those variables whose values have significant effects on the overall economics of the refinery and are inputs to the model whose optimal values are sought by the optimization algorithm. The number of decision variables is equal to the number of degrees of freedom of the model.

III.12. PRICE STRUCTURE

The price structure affects the refinery in relation to both the feed cost and the product revenue. For the feed cost, cheaper crudes mean less expense in purchasing raw materials; however, these cheap crudes may require more processing and treatment to produce salable products. They may also be more expensive to ship. An example is Arab light crude and Arab heavy crude. The light crude has an API gravity of about 33-34; the white product's yield is 63 %. Arab heavy crude has an API gravity of 28 and a much higher sulfur content; the white product's yield is 55 %. Consequently, it is more costly to hydrotreat the sulfur in

the products, requiring the cracking of heavy components to yield the same white products as the Arab light crude. It is, therefore, not surprising that Arab heavy crude is sold for less than Arab light. The effects of crude prices are shown in Figure III-3.

The operation of refineries varies with the seasons, and the price structure is affected by the market demand. For example, the gasoline fetches a higher price in summer when a lot of gasoline is consumed by travelers. Diesel sells for a higher price in winter because the demand for heating oil is high, and diesel can be used to make the heating oil. The two major operation modes are Summer Mode and Winter Mode. Each operation mode has its own price structure.

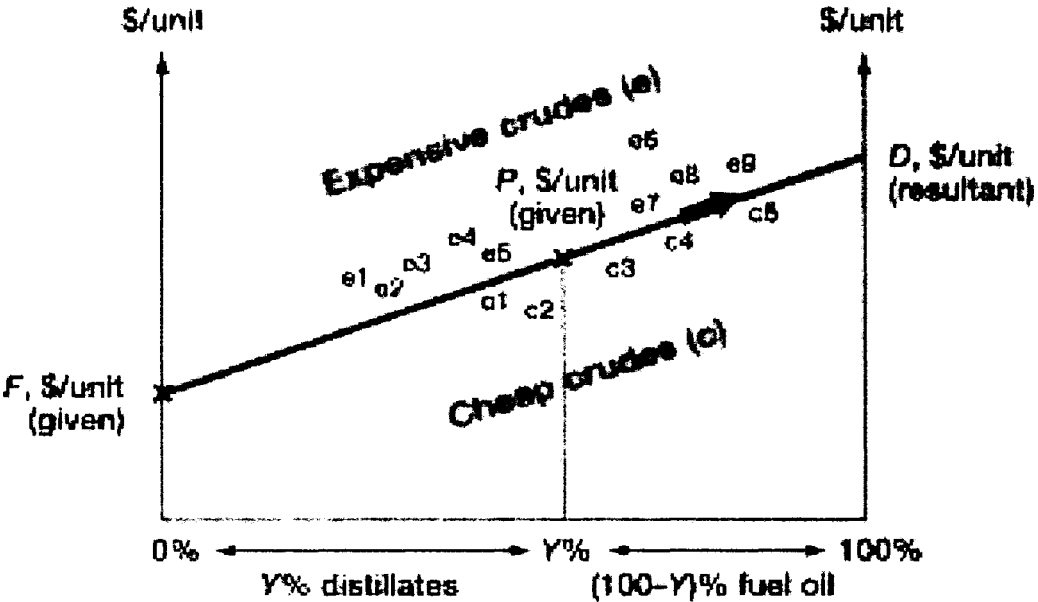


Figure III-3: Effect of Crude Prices on Refineries' Margins [17]

The price gap between gasoline and the diesel increases in summer and decreases in winter. This difference has a great effect on refinery operations, since the price structure directly affects the value of the objective function of refinery optimization.

III.13. SENSITIVITY ANALYSIS

After simulation results were obtained for a certain set of constraints and feed types, sensitivity analysis was carried out to examine the effect of fluctuation of certain variables on the objective function. The sensitivity analysis is the partial derivative of the objective function $\delta\Phi$ with respect to the variable in consideration, δVAR_j , while keeping all other variables constant. A number close to zero indicates a stable objective function with respect to change in a particular variable. In mathematical form this is:

$$\frac{\partial \Phi}{\partial (\text{VAR}_j)} @ \text{all VAR } k \text{ constant } (k \neq j) \quad \text{III-9}$$

During the simulation runs, this was carried out by fixing all variables except one and monitoring its effect on the desired objective. The most obvious candidates for sensitivity analysis were crude and products prices, since these usually have major effects on economics, especially considering the fluctuation in crude prices and product demands. Moreover, other variables such as crude as-

say or unit throughput are not likely to change much. Parameters usually do not have the strong effect on the objective function that variables do, since most of these parameters are virtually constant in the actual refining processes. However, the parameters were checked for sensitivity, especially those that may change with time, such as RON from a CCR unit.

Another category of variables is environmental limitations, since they can affect economics even though it takes years for a regulation to be in effect, whereas, prices can change sharply overnight.

IV OPTIMIZATION ALGORITHMS

This section will discuss the optimization algorithms used in solving the global optimization problem. Since the selected software was Aspen PIMS, this section heavily builds on the Aspen PIMS training manual and other material found in references [29][30][35].

IV.1. SOFTWARE SELECTION AND FEATURES

Simulation runs were carried out using both MATLAB and ASPEN PIMS. Since the model was based on actual refinery data, there was no need for detailed simulations of refinery units. If necessary, PIMS has the capability of communicating with a process simulator, and hence its output can be read by PIMS or sent to other software such as MATLAB as an input.

It was preferred to continue the runs using PIMS since more than 70 % of the world's refineries use it as their primary operations optimization tool. Moreover, its use is convenient for engineers worldwide, since engineers in industry are usually not familiar with C++ or MATLAB programming but are familiar with ready-made simulation packages that are tailor-made for the process industry.

PIMS uses several tools to perform the optimization, including a third party optimization engine known as XPRESS from the Dash Optimization software company [12]. In addition, PIMS uses the same basic chemical engineering

equations needed for mass and material balance. This software has the capability of using various techniques to solve the nonlinear parts of the model. These include Successive Linear Programming, Recursion and Distributive Recursion for the global model case. Each of these methods will be discussed later.

IV.2. LINEAR PROGRAMMING CONCEPTS

As mentioned earlier, LP is widely implemented in the petroleum refining industry as the primary tool for planning and optimization of refining processes and supply and demand allocation. This wide acceptance appears to continue and increase with the use of advanced nonlinear solvers to enhance the LP solution for models with highly nonlinear terms. Since this work is based on LP as the foundation for solving the base model with an extension for solving the nonlinear aspects, LP concepts, strengths and limitations will be discussed. PIMS was used extensively in the simulation of the refineries system. Figure IV-1 shows how PIMS solves an LP model.

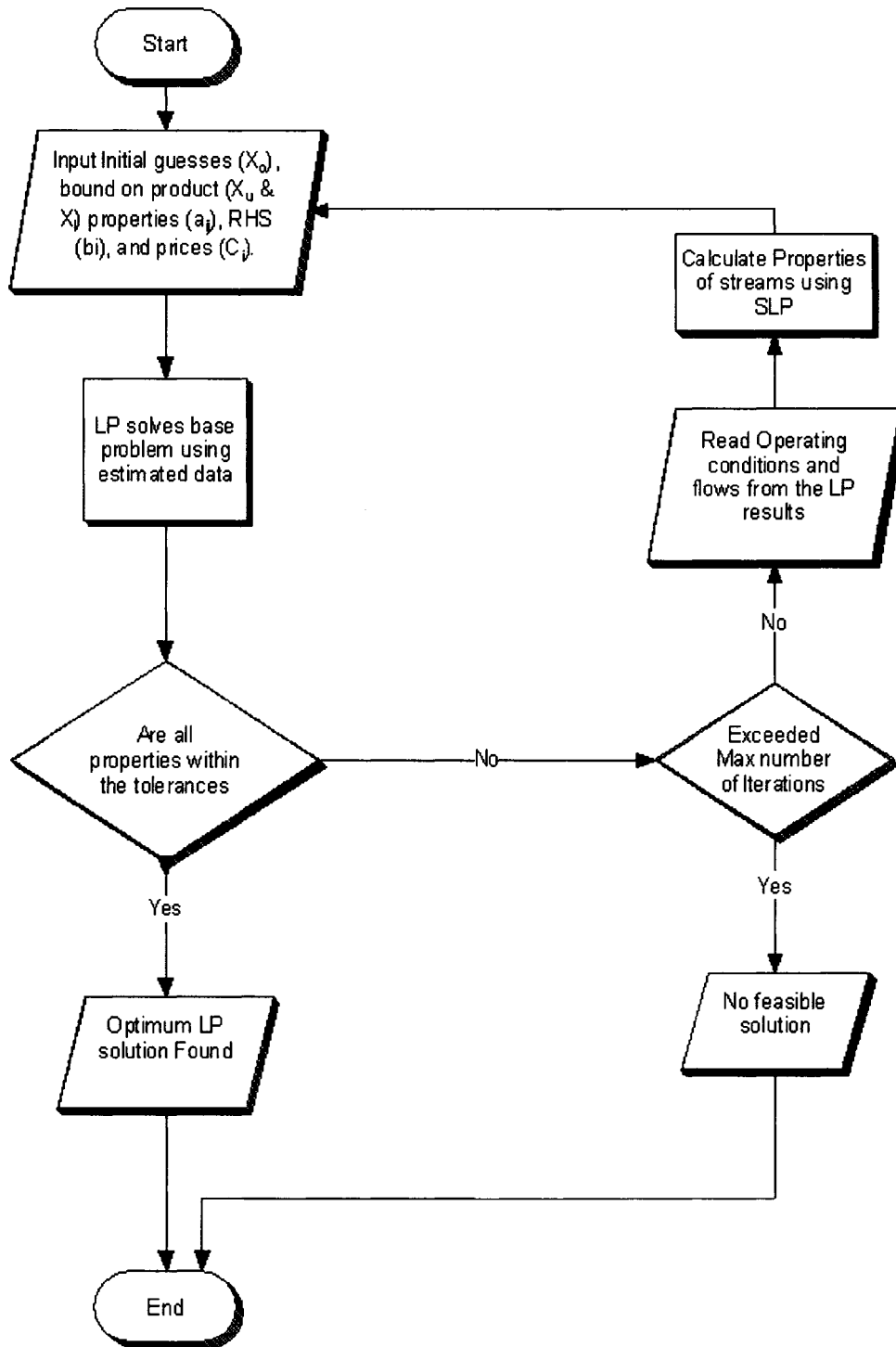


Figure IV-1: Solving an LP model using PIMS

IV.2.1. Definition of Linear Programming (LP)

A linear program model which mathematically models a process such as a refinery, petrochemical plant, distribution system, airline system, a toy factory, etc. in matrix form LP is [24][27] below:

$$\begin{array}{cccccc} X_1 & X_2 & X_3 & X_4 & & \text{RHS} \\ +a_1 & +b_1 & +c_1 & +d_1 & = & M & \text{IV-1} \\ +a_2 & +b_2 & +c_2 & +d_2 & \leq & H & \text{IV-2} \\ X_i \geq 0 & & & & & & \text{IV-3} \end{array}$$

Since there are more unknowns (variables) than equations (constraints), there are infinite number of solutions to the problem or in other words, infinite degrees of freedom. To find the optimum solution, an objective function row is created. This row includes operating costs, feedstock costs, and selling prices of products. The program attempts to maximize the objective function row value, which is calculated as the algebraic sum of each variable's value multiplied by its coefficient in the objective function row. In an LP, variables and constraints must have unique names.

IV.2.2. Constraints (Rows)

Rows represent constraints or equations. The constraints of a process can either be inequalities or equalities. These are needed for the optimization step only if the constraint is limiting at some point; this is referred to as active

constraints. Constraint rows may represent unit capacities, material balances, stream property balances, blending specifications, ratios, utility balances, etc.

IV.2.3. Variables (Columns, Vectors)

These are unknowns in the matrix. For an LP to have more than one unique solution, the number of unknowns has to be more than the constraining rows. The only thing unknown about a column is its activity or final value in the final optimum solution. The LP program assumes that all the other properties of the variable are known, which is not necessarily the case for users of LP. For example, in a refinery, yields and properties of fractionated streams from different crude oils, as well as component blending properties and process unit yields and limits, must all be determined ahead of time for the optimizer to use in solving the problem.

Columns generally represent flow in a process model, i.e., mass flow in tons or pounds, or volume flow in barrels. In some cases it may take several columns to adequately model the stream in a process model, as, for example, in the case of the Platformer where different severity options are available. Each column may have entries in more than one row. Purchases, sales, formula blending, specification blending and process submodeling are among the types of columns of PIMS models are.

LP vector properties must be linked to the actual process properties, such as yield decline as a result of catalyst aging, process unit yield as a function of

feed quality, and physical properties of pools whose composition are calculated by the optimization results.

IV.2.4. Right Hand Side (RHS)

The activity of a row is the sum of each column's activity multiplied by its coefficient in the row. For most rows, the RHS is equal to zero except for capacity rows where the RHS is greater than zero. For equality rows, the RHS must be equal to the activity of the row. The RHS of a less than or equal to row will set the upper limit of the activity of the row, while the opposite is true for the greater than or equal row.

IV.2.5. Ranges

This represents the range that the variable's value can take between the upper or lower limit on a row activity. An example is the unit charge rate, which can range between a maximum throughput to a minimum turndown capacity.

IV.2.6. Matrix Coefficients

Matrix coefficients are the row entries of a column which define the relevant properties of the column, such as price, cost, yield, physical properties, utility consumption, and capacity consumption. For example, a charge vector for a crude unit will have coefficients indicating how a specific crude oil will be fractionated in a specific crude unit, while a reformer severity vector will have coeffi-

cients showing a specific yield pattern for that severity, together with specific capacity consumptions as they relate to that severity.

IV.2.7. Bounds

Bounds are used to set upper and lower limits on the activity of a column in the optimum solution. By definition, the upper bound of all columns is plus infinity and lower bound is zero unless these limits are changed by the user.

IV.2.8. Shadow Pricing: Rows (π)

Shadow pricing is an important concept in an LP optimization. It demonstrates the benefits and costs of going an additional step from the optimum. For example, if the optimum production level of a refinery product is 20 KBPD, shadow pricing will show the benefits of producing an extra barrel per day and its effect on the objective function. Hence, it is a type of sensitivity analysis.

Pi value (π) represents the rate of change in objective function when the RHS of a row is increased. Pi values are therefore partial derivative of the objective function with respect to a specific row [29][30],

$$\text{Pi} = \frac{\partial \text{Objective function,}}{\partial \text{Row Name}} \quad \text{IV-4} \\ \text{@all other variables constant}$$

Shadow price Pi is the value of the next increment of this material. The size of the increment is indefinite and can range from infinitesimal size to a large increment. The Pi value sign is determined by the sign convention used in the

associated row and the sign convention of the objective function. Shadow pricing was extensively used in this model and is a PIMS output.

IV.2.9. Columns ΔJ

Columns ΔJ (DJ) represents the change in the objective function value for an incremental change in column activity. DJ is zero for all basis columns, which reflects the fact that the cost of producing the next increment and the product value of the next increment exactly balance each other and the slope is zero. The DJ of a column that has an entry in the objective function row is the difference between this entry and the incremental value of the column in a solution [29, 30].

IV.3. PROBLEMS WITH LP

There may be some problems when using linear relationships to model nonlinear process operations. This is particularly observed in processes with inherent nonlinearity and high component interaction such as product blending in which activity coefficient and blending indices play a big role. The following are some examples of such cases.

IV.3.1. Additive Concentration Versus Response

This phenomenon is typically seen in blending TEL into gasoline to improve its RON. The response curve is approximated utilizing tangents to the response curve. These are slopes that approximate the response of blend to addi-

tive [29, 30]. Figure IV-2 illustrates this relationship. However, in this research, no TEL blending was assumed since all work was done on unleaded gasoline.

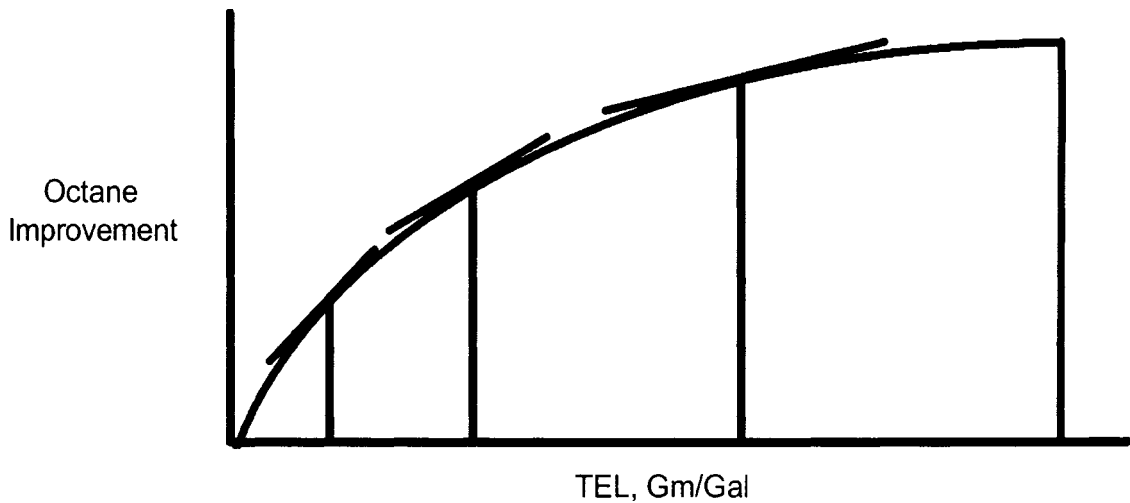


Figure IV-2: Additive Concentration Versus Response [30]

IV.3.2. Synergism or Antagonism

This is a common problem in blending. Usually when two or more streams are blended together, the resulting blend may not have the same properties as when the streams are mathematically ratioed in the same proportion as the blend. Antagonism occurs when the properties of the actual blend are less than the calculated properties. Synergism takes place when the actual blend properties are greater than the calculated properties [29, 30]. Figure IV-3 shows these two cases, which have been widely observed in the results, especially in gasoline blending. For example, blending 10 KBPD of Reformate with 10 KBPD FCC gasoline yields less than 20 KBPD of final gasoline product.

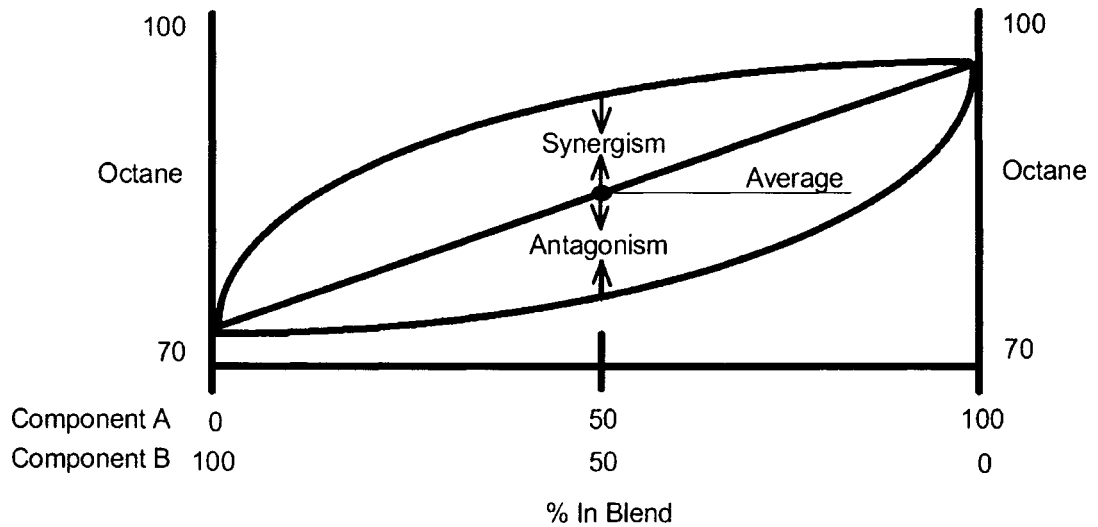


Figure IV-3: Synergism or Antagonism [30]

IV.3.3. Yield Loss Over Time

This is a typical problem found in refineries where catalysts such as reforming or Hydrocracking catalyst is deactivated over time. As the catalyst activity decreases, the yield from the process unit deteriorates. LP can only recognize one set of yields at a time. Yield changes over time must be related to the LP by updating appropriate yield coefficients. A common example is Platformer's yield loss with catalyst aging [29, 30]. Figure IV-4 illustrates this phenomenon. As was mentioned in the assumptions, the model did not account for the catalyst's deactivation since this is beyond the scope of this work, which concentrates on the global optimization of refineries at any given point of time, while catalyst deactivation is more related to detailed refinery optimization over a long period of time.

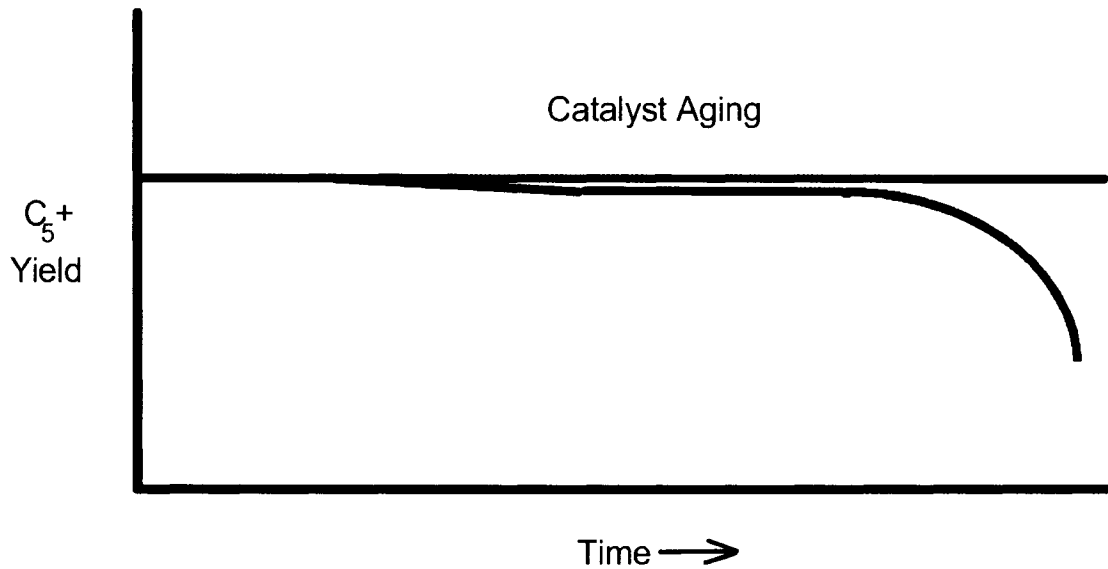


Figure IV-4: Yield Loss Over Time [30]

IV.3.4. Column Arithmetic

For LP models, we can neither multiply nor divide one column by another, nor can we raise a column activity to an exponential power. Distributive recursion can overcome these limitations and the problem then becomes using a non-linear approach to solve linear equations.

IV.3.5. Pooling of Streams

In a process model LP, many streams are combined to form intermediate streams (pools) which are fed to a process unit. Data for the pooled stream must be supplied in order to reach a solution. However, the composition of the pooled stream is not known until after the optimum solution is reached.

For example, in the production of alkylate from both C₃ and C₄ olefins, C₃ alkylate is six numbers below C₄ alkylate RON. The question therefore arises as to what octane should be assigned to the combined alkylate, since the composition of the olefin feed stream is unknown. In this situation, distributive recursion comes into play by allowing the LP matrix coefficients to be updated automatically based on the column activities of a prior solution. This is an iterative process that continues until the specified tolerance is met, the solution is said to have converged, and further changes cannot improve the solution [29, 30].

IV.4. CONSTRAINED MULTIVARIABLE SEARCH METHODS

There are six procedures for solving constrained nonlinear optimization problems. The most successful of these are successive linear programming, successive quadratic programming, and the generalized reduced-gradient method. The other three methods are penalty and barrier function methods, augmented Lagrangian functions, and the method of feasible directions. These methods have not proved to be as useful, especially in solving problems with more than twenty variables. Of these methods, only successive linear programming does not require an unconstrained single or multivariable search algorithm.

IV.5. SUCCESSIVE LINEAR PROGRAMMING (SLP)

In this section, Successive Linear Programming (SLP) will be analyzed in detail since it is the algorithm PIMS uses to solve the nonlinear terms in the LP

model. As will be discussed below, SLP has proved to be the best nonlinear algorithm to solve very major refining problems with acceptable accuracy and speed.

Pike [28] described that Griffith and Stewart of the Shell Oil Company originally proposed and tested this procedure on petroleum refinery optimization; they termed it the method of approximate programming (MAP). This method uses linear programming as a search technique. The starting point is selected, and the nonlinear parts in the economic model and constraints are then linearized around this point to yield a linear problem that can be solved by the Simplex Method or its extensions. The point from the linear programming solution can be used as a new point for linearizing the nonlinear problem, and the process is repeated until the specified tolerance or a stopping criterion is met. The algorithm flow chart is shown in Figure IV-5.

This procedure does not require safeguards for functions that are mildly nonlinear. For larger problems having high numbers of nonlinear variables with high degrees of nonlinearity, it is necessary to bind the steps taken in the iterations to insure that the economic model improves, the values of the independent variables remain in the feasible region, and, of course, that the procedure converges to the optimum. Safeguards are the bounds on independent variables specified prior to solving the LP problem, which result as additional constraint equations. If the bounds are set too low, the procedure will move slowly toward the optimum solution, while if they are set too high, unfeasible solutions may be generated [4]4, 5, 28].

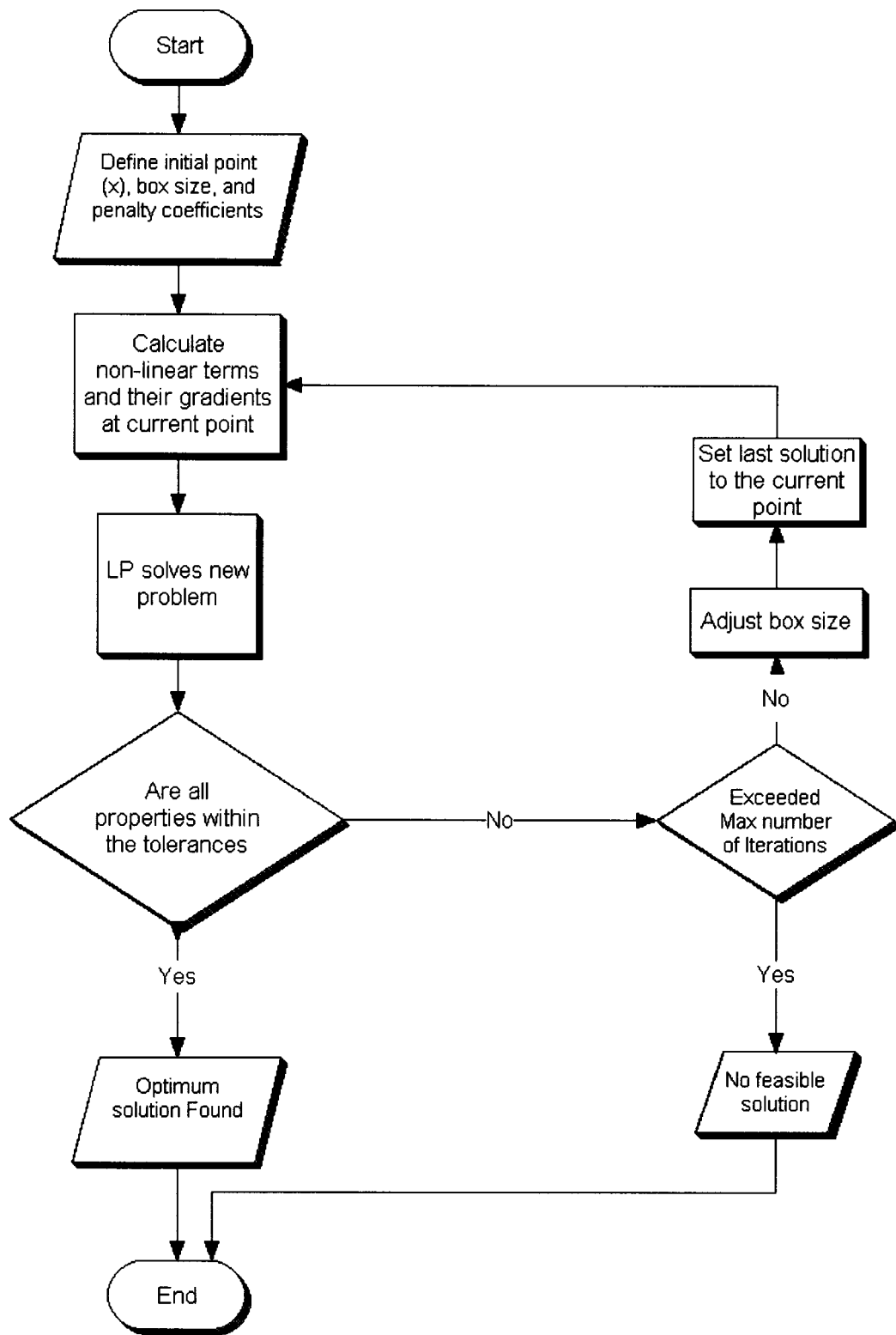


Figure IV-5: Successive Linear Programming Flow Chart

The general formula for successive linear programming is:

$$\text{Optimize: } y(x) \quad \text{IV-5}$$

$$\text{Subject to: } f_i(x) \leq b_i \quad \text{for } i = 1, 2, \dots, m \quad \text{IV-6}$$

$$u_j \geq x_j \geq l_j \quad \text{for } j = 1, 2, \dots, n. \quad \text{IV-7}$$

The upper and lower bounds shown are independent variables. The nonlinear economic model $y(x)$ and the constraints $f_i(x)$ can be linearized around a feasible point x_k to yield:

$$\text{Optimize} \quad \sum_{j=1}^n C_j \Delta X_j = Y - Y(X_k) \quad \text{IV-8}$$

$$\text{Subject to} \quad \sum_{j=1}^n a_{ij} \Delta X_j \leq b_i - f_i(X_k) \quad \text{IV-9}$$

$$U_j - X_{jk} \geq \Delta X_j \geq l_j - X_{jk} \quad \text{IV-10}$$

$$\Delta X_j = X_j - X_{jk} \quad \text{IV-11}$$

$$a_{ij} = \left[\frac{\partial f_i(X_k)}{\partial X_j} \right]_{\text{all } X_k, [k \neq j]} \quad \text{IV-12}$$

$$C_j = \left[\frac{\partial Y(X_k)}{\partial X_j} \right]_{\text{all } X_k, [k \neq j]} \quad \text{IV-13}$$

For $i = 1, 2, \dots, m$; $j = 1, 2, \dots, n$

This is a linear programming problem. The values of Δx_j can take on either positive or negative values, depending on the optimum solution. Since a simplex algorithm does not accept negative values for Δx_j , a change of variables was made by Griffith and Stewart, as follows [28]:

$$\Delta x_j = \Delta x_j^+ - \Delta x_j^-$$

where

$$\begin{aligned} \Delta x_j^+ &= \Delta x_j \quad \text{if } \Delta x_j \geq 0, \\ &= 0 \quad \text{if } \Delta x_j < 0. \end{aligned}$$

$$\begin{aligned} \Delta x_j^- &= -\Delta x_j \quad \text{if } \Delta x_j \leq 0, \\ &= 0 \quad \text{if } \Delta x_j > 0. \end{aligned}$$

These values are then substituted in the equation above to give a linear programming model.

The bounds on the upper and lower limits of variables are specified by $(u_j - x_{jk})$ and $(l_j - x_{jk})$. The value of the next point for carrying out the linearization is given by

$$x_{jk+1} = x_{jk} + \Delta x_j^+ - \Delta x_j^- \quad \text{IV-14}$$

This is now another linear programming problem where the independent variables are Δx_j^+ and Δx_j^- . The value of the bounds u_j and l_j may have an effect on the rate of convergence of the algorithm.

The successive use of linear programming has been successful in large plants where, in most cases, the procedure has been used by companies that have invested extensively in the development and use of large linear programming codes for plant optimization and a corresponding amount of effort in large simulations of key process units for prediction of performance and yields. Petroleum refining is one of the broadest fields for SLP, in which linear programming is used for refinery optimization. In addition, simulations and correlations have been developed for processes such as catalytic cracking, reforming and distillation [14, 28]. The model hierarchy of combining all of these tools is shown in Figure IV-6 [21].

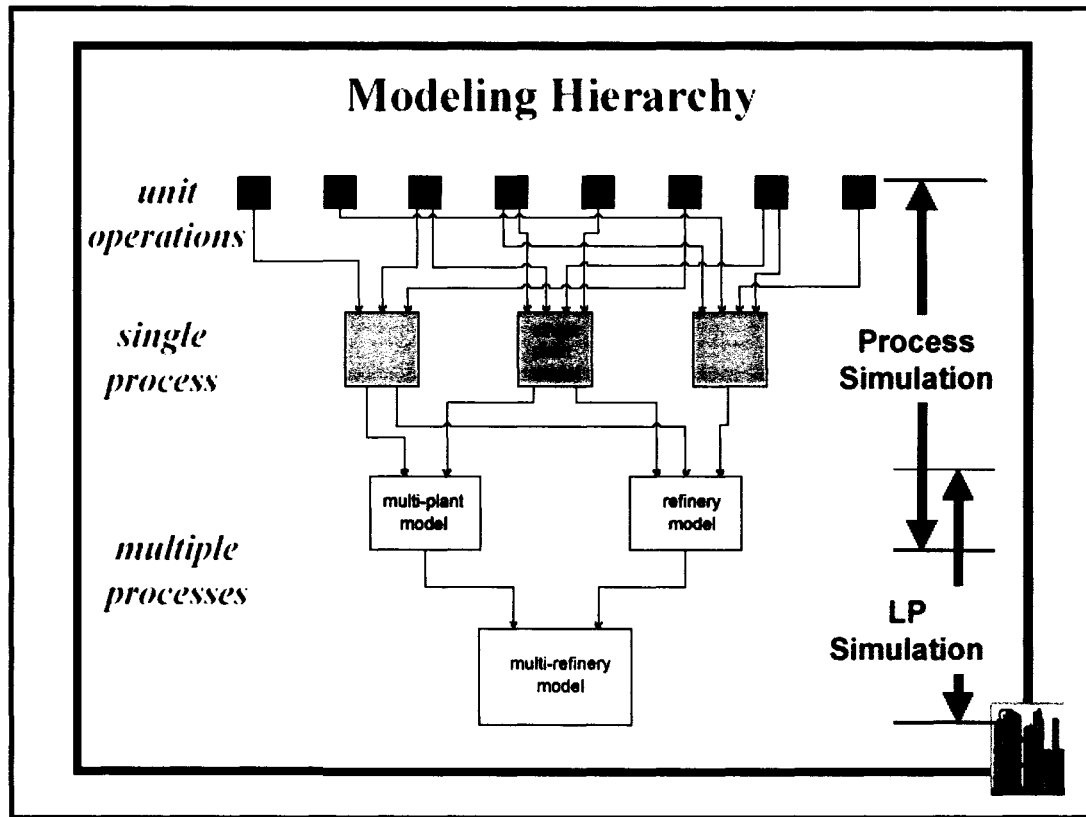


Figure IV-6: Model Hierarchy [21].

IV.6. XPRESS-SLP

XPRESS is a solver for non-linear and mixed integer non-linear programming problems. It uses successive linear approximations that have been developed from techniques used in process industries and is capable of solving huge problems with thousands of variables. XPRESS is provided by a company called Dash Optimization [12]. PIMS utilizes XPRESS as the engine for solving both LP and mixed integer problems.

For LP problems, the engine gives the choice of using either primal, dual or the Newton barrier solution algorithm. The first two are simply well-known

versions of the famous Simplex method, which has been the basic optimization method of the refining and petrochemical industries for decades, while the third is a version of the known interior point method presented by Kramakar in 1985. However, all of the optimization runs in this research were carried out using the Simplex primal method—i.e., the default method—in order to obtain consistent comparisons between all runs.

IV.7. DELTA BASED MODELING

In this section, Delta Based Modeling (DBM) will be discussed. This is a technique used by most optimization software, including PIMS to account for the problem of dependency of the physical properties of streams on the composition of feed. DBM had proved to be very useful in solving very large refining problems with thousand of variables.

Delta Based Modeling is a linear programming technique used to predict yields or properties of process units and their products in situations when these yields and properties are a function of feed quality. For example, in a Platformer, the Reformate yield will increase with higher feed Naphthenes plus aromatics (NPA), and vice versa [30]30, 35].

In most LP models, the feed is a pool of streams whose composition is unknown and must be determined by the optimization process. Because we do not know the composition of the feed pool, the properties of the feed to a unit are likewise unknown. DBM is useful in such cases when combined with the Distributive Recursion (DR) technique. Using DR, we can estimate the required

feed pool properties, and when the solution has converged, we will have the correct properties for accurately predicting the product yields and properties.

To implement DBM, a feed quality parameter is defined which can be easily measured and accurately predicts product yields and/or properties. An example of this relationship is shown in Figure IV-7.

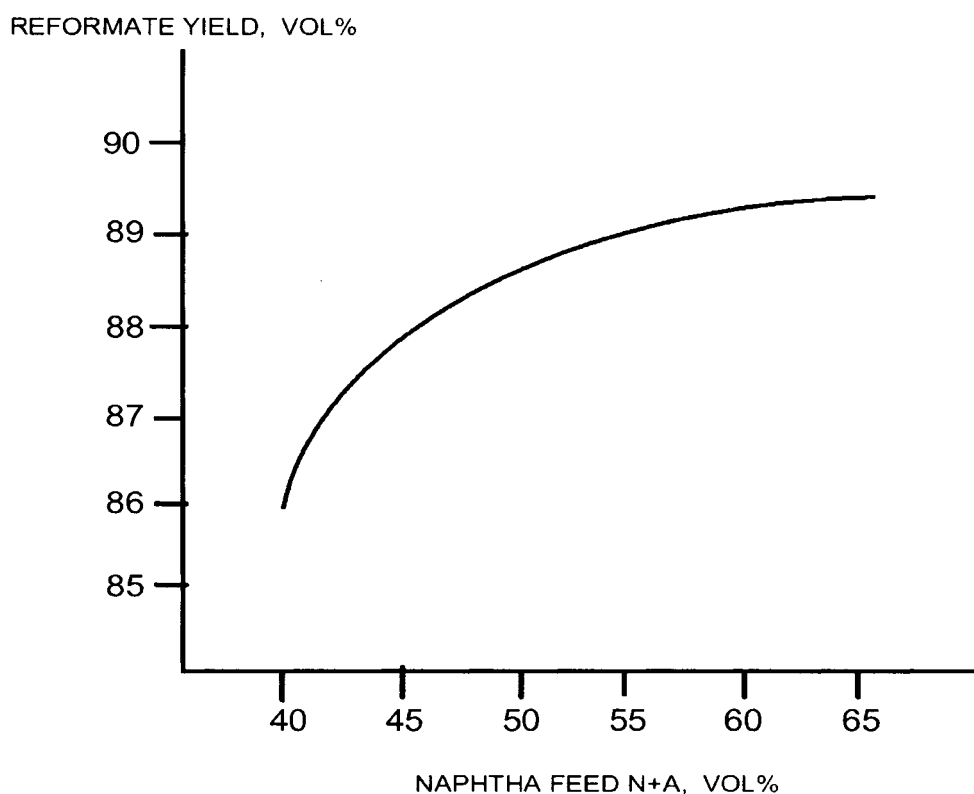


Figure IV-7: Reformate Yield Versus Naphtha Feed N + A (NPA) [30]

IV.8. RECURSION

Recursion is the process of solving a model, examining the optimum solution with an external program, calculating physical properties, updating the model

using the calculated properties, and then solving the model again. The process is repeated until the specified tolerances are met.

Recursion was introduced to solve a problem when using linear programming for refining system modeling. When a model is built to represent a process such as a refinery, there are data in the model that need to be estimated. These usually relate to the physical properties of materials used in the refinery to produce products.

For example, premium gasoline is blended in a refinery to meet certain specifications for RON, RVP, and distillation. Therefore, when blending data are provided for each of the blend components to be used by the optimizer to blend the final gasoline product, such data have to be estimated if not available. Some of these data are dependent on other factors such as feedstock quality and operating conditions such as the cut point for each material out of the crude unit, the severity at which the reformer was run, and the ratio of C₃ olefin to C₄ olefin in the feed to the Alkylation unit. Inaccurate estimation of such data can lead to inaccurate solutions.

IV.8.1. Recursion Mechanism

The recursion procedure is illustrated in Figure IV-8 [30]. First, the optimizer solves the model containing the estimated data. Once the model is solved, an external computer program calculates the physical property data being used in the model from the optimum solution. The external program then examines the optimum solution produced by the optimizer and calculates the physical

property data of the crude fractions, using the composition of the crude slate in the solution. These data are then inserted into the LP matrix updating the estimated data with more accurate data. The model is then resubmitted to the optimizer and the cycle continues until the changes in the calculated data are within the specified tolerances.

IV.9. DISTRIBUTIVE RECURSION

Distributive Recursion (DR) is a non-linear convergence technique used in linear programming to model nonlinearities by approximating them with linear segments and updating the LP matrix during a recursion pass. Distributive recursion allows the properties of a pool to be continuously updated throughout the optimization process to match predefined tolerances. In this work, DR was used throughout the simulation cases in the global optimization runs.

IV.9.1. Distributive Recursion Mechanism

After solving the matrix using initial physical property estimates, new values are computed from the solution and inserted into the matrix for another LP solution. The major difference between Distributive Recursion (DR) and simple recursion is the manner of handling the difference between the guess and the calculated physical property data from the optimizer solution. This difference is termed the "error," since error appears in the model when the user guesses at the physical properties of recursed pools in an LP model because guesses will not be exact [30].

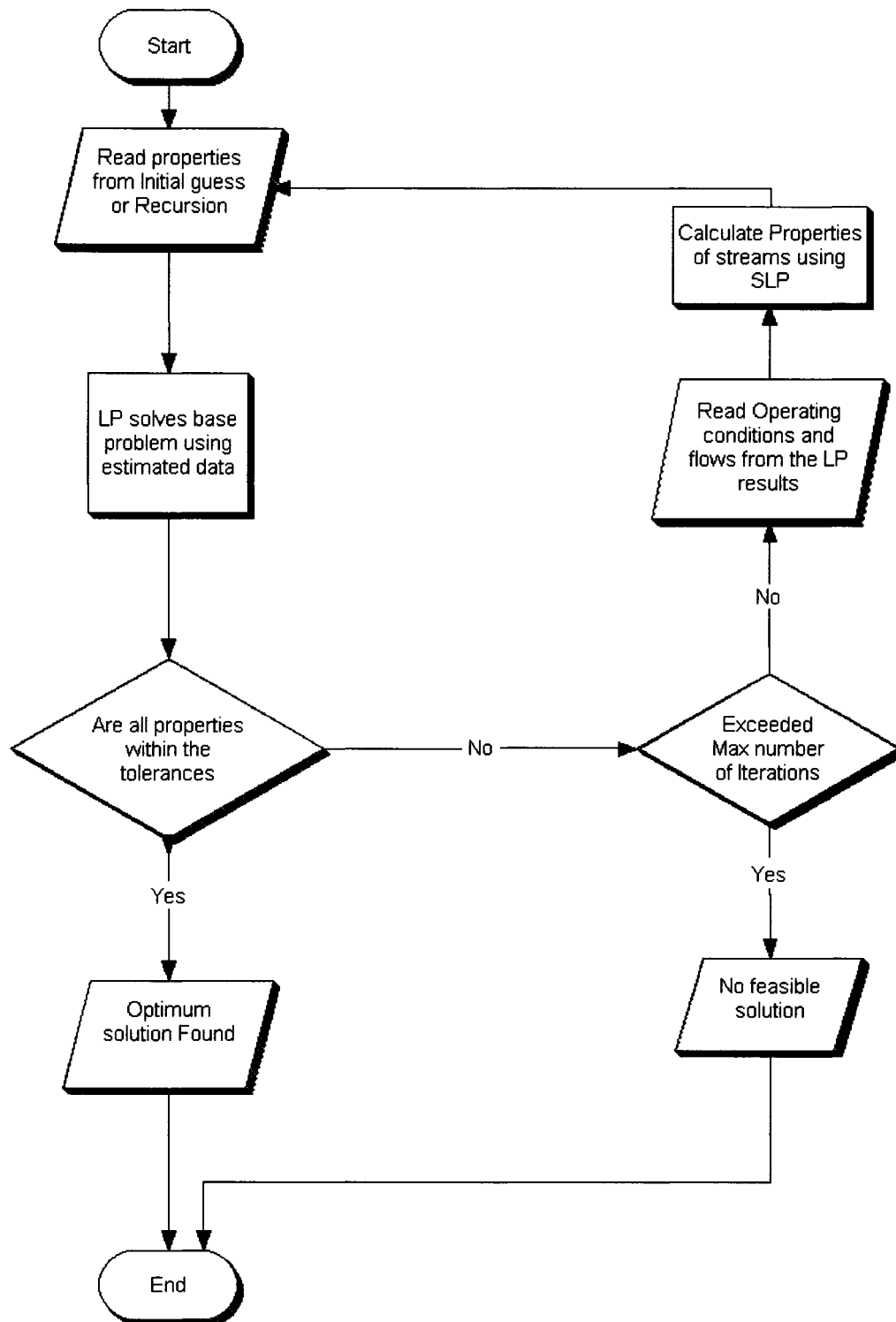


Figure IV-8: Recursion Flow Chart

The distributive part of Distributive Recursion utilizes the fact that this error is distributed to the location where the quality is being used. Thus, downstream locations where the recursed pool's physical properties are being used have visibility back to the pool source and are able to evaluate, through this error-handling model structure, the benefits and penalties of alternate operations. On the other hand, the upstream producer of these pool properties is able to evaluate the benefits and penalties of alternate quality operations on the downstream use of the pools.

An example of distributive recursion is the gasoline-blending section of the LP model. If a guess of 96 RON is assigned to the Platformer Reformate, the blending section is able to look upstream and evaluate the economic benefits or penalties of changing the Platformer operation to produce a different RON Reformate. Simultaneously, the Platformer is able to look downstream to evaluate the economic benefits or penalties associated with blending if a change is made in the Platformer operation to produce a different RON Reformate. The distributive recursion matrix structure provides visibility from the source of a recursed pool to its terminal, and vice versa [30].

IV.10. MATLAB OPTIMIZER

For the MATLAB runs, the Optimization Toolbox was used to solve the multi objective single refinery optimization problem. The command "linprog" solves the linear programming problem. linprog is a variation of the well-known

Simplex method of linear programming. It finds an initial feasible solution by first solving another linear programming problem.

The problem can also be solved by using the MATLAB large-scale method based on Linear Interior Point Solver, which is a variant of Mehrotra's predictor-corrector algorithm [26]. However, in the simulation runs on MATLAB, only the LP programming commands were used. No nonlinear functions were employed to compensate for the nonlinearity of some of the variables. This was done deliberately in order to compare the raw results from a straight-through LP program with a more sophisticated algorithm that uses SLP and DR for the calculations of the nonlinear parts. As will be discussed later, even though there was a clear difference in the results, this difference was small and all runs followed the same trend. This is due to the fact that there were not many nonlinear terms in the comparison model. As mentioned earlier, a high degree of nonlinearity usually appears in blending problems.

V A DESCRIPTION OF REFINERIES AND MARKETS SYSTEM

V.1. A DESCRIPTION OF THE REFINING SYSTEM

The model consisted of seven refineries. Five of these are mainly domestic refineries with variable capabilities for exporting excess products to other refineries or international markets. These refineries were built with the view of supplying local markets; consequently, there are limitations on the type and quality of products they are able to produce. For example, many of them cannot produce Reformulated Gasoline RFG. The other two refineries are export, state-of-the art refineries, as will be described below. Table V-1 gives a summary of the major process units and capacities for each refinery.

V.1.1. Export Refinery # 1

This is a state-of-the-art refinery geared toward providing products for international markets, notably the US and Europe. Consequently, this refinery is able to produce the most stringent product spec available, such as 50 PPM sulfur diesel, 99 RON gasoline, and reformulated gasoline RFG. At the same time, it can provide products to the domestic market at the expense of exporting them to

international markets. The refinery has an FCC unit, a CCR, an Alkylation unit, and online blending facilities. It is considered a fuel refinery, more specifically a gasoline refinery.

V.1.2. Export Refinery # 2

This is also a state-of-the-art export refinery, primarily geared toward providing chemical feed stock, such as Benzene-Toluene-Xylene mixture (BTX) and chemical feed naphtha to nearby petrochemical plants. However, the facility is capable of producing specialty products and high quality fuels. This refinery is considered to be a petrochemical-oriented refinery.

Table V-1: Summary of Refinery Processes

	Crude Ca- pacity, KBPD	Condensate	Reformer	CCR	FCC	HC	DHT
Export refinery # 1	200		N	Y	Y	N	Y
Export refinery # 2	200	N	N	Y	N	Y	Y
Domestic Refinery # 1	300	200	Y	Y	N	Y	Y
Domestic Refinery # 3	80	N	Y	N	N	N	N
Domestic Refinery # 4	450	N	N	N	N	N	Y
Domestic Refinery # 5	210	N	Y	N	N	N	Y

V.1.3. Refinery # 1

This is a domestic refinery that was built to provide petroleum products, mainly fuels, to the eastern and central regions of the country in the study. The demand in these two regions is mainly for distillate fuels and fuel oil. The refinery is a large one, with a crude capacity of 300 KBPD, 200 KBPD condensate splitter, CCR reformer, Hydrocracker and fixed bed reformers, together with sulfur plants and distillate Hydrotreaters. Although it is not state-of-the-art, this refinery is considered a complex refinery; for example, it does not have a FCC unit nor is it capable of producing specialty gasoline such as RFG.

V.1.4. Refinery # 2

This is a domestic refinery that was built to provide petroleum products, mainly fuels, to the central region of the country. The demand in this region is mainly for distillate fuels. The unique thing about this refinery is that it is inland and does not have access to open seas, nor is it connected to a rail system. This can be a bottleneck in exporting excess products that cannot be absorbed by the local market; for example, the heavy part of the oil that cannot be further cracked is transformed into asphalt and fuel oil. In a country that does not need fuel oil for heating purposes and lacks tankers and bunker markets, the only use of fuel oil is the refinery's internal fuel usage and nearby power plants or local industries. If these markets are unable to absorb the production of its fuel oil, the refinery shifts to asphalt production. Due to the limited market for asphalt, this refinery may reach a point at which it needs to reduce the refinery charge rate to

avoid having unsellable products. The refinery is considered a high complexity refinery with two crude units, two Hydrocrackers, an Isomerization unit, distillate Hydrotreaters and a DMO unit.

V.1.5. Refinery # 3

This is a very small domestic refinery that was built to provide petroleum products, mainly fuels, to parts of the region. The demand in this area is mainly for gasoline; consequently, this refinery is the only domestic refinery having a catalytic cracking unit FCC. The refinery has a complicated objective function structure, since it is interconnected to a lube refinery and a bulk plant. The marine terminal of this refinery is also used in transferring products to the bulk plant, since the refinery cannot meet the entire demand for that area. The refinery is very small, of medium complexity, having an effective throughput of 80 KBPD crude distillation, a 20 KBPD FCC unit, 3 KBPD Platformer, and no distillate or kerosene Hydrotreaters. This constrains the refinery to produce low sulfur diesel, as will be seen in the environmental section cases.

V.1.6. Refinery # 4

This is a mixed purpose refinery, a huge facility with one crude unit having a capacity of 450 KBPD. Despite its size, the refinery has only one distillate Hydrotreater, unit and it does not have any upgrading or cracking units, which makes it a major exporter for intermediate products such as LPG, chemical feed naphtha, and straight run fuel oil. Actually this fuel oil is very valuable since it

can be further used as a feed to a FCC unit to produce high quality fuels. However, with such a huge size refinery, any expansion or addition would require substantial investment involving significant risk factors.

V.1.7. Refinery # 5

This is a domestic refinery that was built to provide petroleum products, mainly fuels and lube refinery feedstock, to the largest fuel market which is the western region that consists of approximately seven markets. This refinery is a simple hydroskimming facility having only a Platformer and distillate Hydrotreater units.

V.2. MARKETS AND OTHER LOCAL MODELS IN THE GLOBAL MODEL

In addition to refineries, the model consisted of 14 bulk plants, 36 markets, terminals, pipelines and export hoppers. Most of the bulk plants are modeled in the program as depots. The model had 36 markets of which 5 are long term storage facilities. Some of these markets are very small and in remote areas. On the other hand, some metropolitan areas typically have two or more markets that are usually very large. Even though they can obtain products directly from other bulk plants, a bulk plant is usually tied to each of these markets.

In our modeling, only refineries and mixed terminals are of importance in relation to the objective function, and these are modeled in detail. For proprietary

reasons, export refineries are not modeled in detail, and there is no detailed information concerning process operating conditions as is the case for the domestic refineries. Instead of having a detailed sub-model for each process unit, the model includes the yield table for each refinery, which serves as a calculator for the feeds required to produce a certain blend. This works well for our purposes. The model can request the product, supply the required feed to these refineries, and utilize only the share of the company in these refineries.

VI MULTI OBJECTIVE-SINGLE REFINERY OPTIMIZATION

VI.1. INTRODUCTION

Multi objective-single refinery optimization is the first step in carrying out the overall optimization process. Even though the title may indicate that this is applicable only to a single refinery system, it differs from the regular refinery optimization found in the literature in the following ways:

1. It focuses on multi objectives rather than a single objective. This includes economic, environmental, safety and catastrophic failure effects, or simply a custom objective such as providing the feed for a nearby petrochemical complex that requires stringent feed characteristics regardless of other objectives such as economics or utilization. In cases where the refinery is under environmental pressure, the objective may just be to reduce the total emissions from the refinery.
2. It is a first step in the multi refinery system. The difference is that it is operational in a single refinery but utilizes the same supply/demand chain. Other refinery optimization models usually start from the refinery as the base system and thus assume that the refinery has complete flexibility in selecting the feeds and products structure. In our case, this is not neces-

sarily true since the refinery is a part of the global system and can therefore have only what is available to it from other sources in the grid. It also can produce only what the chain can accept.

VI.2. CASE STUDY

A case study was done on a refinery that has flexibility in having different crude charges and products as follows:

VI.2.1. Process Description

- Crude type: Arabian light AL or Arabian heavy AH crudest.
- Straight run crude cuts: Naphtha (N), Kerosene (K), Diesel (D), and Reduced Crude (R).
- Conversion units: FCC and CCR
- Final products: Premium Gasoline (PG), Regular Gasoline (RG), Diesel (DSL) and Fuel Oil (FO)

The model has 32 streams (feeds, intermediate products and final products) and 37 constraints. The model was simulated using the MATLAB linear programming solver. In most cases, the model converged to a solution.

VI.2.2. Constraints

Below are some of the constraints used, including the constraints mentioned earlier:

Capacity constraints

	Min	Max
Crude charge, KBPD		
Arab light	0	100
Arab heavy	0	100
<u>Process units capacities, KBPD</u>		
CCR	0	25
FCC	0	25
<u>Final Products, KBPD</u>		
Regular Gasoline	10	100
Premium Gasoline	10	100
Diesel	10	100
Fuel Oil		

This can be written as:

$$CH = \sum (\text{Feed}_k \cdot \text{wt}_f),$$

where CH is the crude charge to the crude distillation unit CDU,

$$N \geq 0.18 \text{ AL}$$

$$N \leq 0.26 \text{ AL Etc.}$$

Full constraints are in spreadsheet format since it is easier to analyze and to input into MATLAB. This spreadsheet is shown in Table VI-1 and Table VI-2.

This spreadsheet was further rearranged to be in the standard form for linear programming, that is, in the form of

$$H(X) = 0;$$

$$g(X) \leq 0$$

Table VI-2: Constraint Spreadsheet for Product Finishing

	FCC				Platformer			PREMIUM GASOLINE				REGULAR GASOLINE				CONST	RHS			
	MCB	FCCFG	FCCLPG	FCCGASO	HSRPLT	PLAT	PLTLPG	LSRPG	PLATPG	HSRPG	FCCPG	PG	LSRRG	PLATRG	HSRRG			FCCRG	RG	
OBJECTIVE FUNCTION																				
Prices		-40										-37								
FCC	Fuel oil blending cons	1															=	0		
	Production	1	1	1	1													≤	0	
	Gasoline balance				-1						1					1		=	0	
	Vol.expansion set at 5%	1		1	1													=	0	
	Gasoline Yield				1														≤	0
	MCB Yield	1																	≤	0
Platformer	Naphtha Splitter bal					1		1	1			1	1					=	0	
	Balance					-1	1	1										≤	0	
	Reformate yield					-0.82	1											≤	0	
	Capacity const					1.00												≤	25000	
	Reformate balance						1		-1					-1				=	0	
PREMIUM GASOLINE	MIN PRODUCTION										1							≥	10000	
	BLENDING CONST							1	1	1	1	-1						=	0	
	OCTANE							-78.5	-104	-65	-94	93						≤	0	
	RVP							18.4	2.6	6.5	6.9	-12.7						≤	0	
	MIN PRODUCTION																1	≥	10000	
REGULAR GASOLINE	BLENDING CONST											1	1	1	1	-1		=	0	
	OCTANE											-78.5	-104	-65	-94	87		≤	0	
	RVP											18.4	2.6	6.5	6.9	-13		≤	0	

To explain how these constraints were set, let us take the naphtha yield as an example of the constraints in this table. In Table VI-1, there is a row entitled “naphtha yield.” In this row, the following numbers appear under each column respectively: -0.22, - 0.15, and 1 and 0 under the columns ALT, AHVY, N and RHS. ALT and AHVY stand for Arab light and Arab heavy crudes, respectively. The constraint sign is less than or equal. When multiplying this matrix, the resultant constraint inequality is:

$$\text{Naphtha yield: } -0.22 * \text{ALT} - 0.15 \text{ AHVY} + \text{N} \leq 0,$$

or in a more practical form:

$$\text{Naphtha yield: } 22 \% \text{ of ALT crude} + 15 \% \text{ of AHVY} \leq \text{N yield.}$$

These percentages refer to the amount of naphtha in each stream. Thus, Arab light crude has a naphtha content of 22 %, while the heavier Arab heavy crude has only 15 % naphtha yield and the stream N has 100 % naphtha composition. The less than or equal sign shows that these are the maximum limits of naphtha that can be extracted from each crude. The percentage can be less but not more; otherwise, it will lead to an off-spec product. The only product that differs from this is the reduced crude, since it is not affected by the amount of white products dumped into it. In fact, this will raise its price.

VI.2.3. Linear Programming Results

After writing the constraints and rearranging them in a MATLAB-readable format, optimization runs were done using the built-in optimization model in MATLAB, which uses an advanced Simplex approach. The variables were manipulated to illustrate the effects of some key variables on the optimization process. The two main variable categories were price and capacity limits, with the latter controlling the optimization since the optimizer tends to produce a variable set that will maximize the objective function. Product specifications and capacity limits are therefore necessary in order to make sure that one obtains a reasonable solution. Table VI-3 summarizes the simulation results, which are discussed below.

Table VI-3: LP Simulation Results

Case Number	1	2	3	4	5	6
Case Description (Flow is in KBPD)	Base Case	Heavy crude Pe- nalized by 1\$	Base Case + PG Price = \$ 44	Diesel and PG Prices set @ \$ 40	All White Products set @ Same Prices	No lower Bound on Diesel or PG but Only on RG
ALT	0.0	0.0	0.0	0.0	100.0	16.2
AHVV	100.0	1.0	100.0	100.0	0.0	83.8
CH	100.0	1.1	100.0	100.0	100.0	100.0
N	15.0	0.2	15.0	15.0	22.0	16.1
K	7.1	0.1	7.1	7.1	9.9	7.2
D	30.0	0.3	30.0	30.0	25.0	29.2
R	47.9	0.5	47.9	47.9	43.1	47.5
VTB	28.7	0.3	29.4	27.7	33.1	31.7
VGO	19.2	0.2	18.5	20.2	10.0	15.8
VGOFO	19.2	0.2	18.5	20.2	10.0	15.8
KFO	1.6	0.0	1.6	1.6	5.3	1.8
KDP	5.5	0.1	5.5	5.5	4.6	5.4
DSL	35.5	0.4	35.5	35.5	29.6	34.6
FO	49.5	0.5	49.5	49.5	48.4	49.3
HSRPLT	9.2	0.1	9.2	9.2	11.1	6.3
PLAT	7.6	0.1	7.6	7.6	9.1	5.2
PLTLPG	0.8	0.0	0.8	0.8	1.9	0.6
LSRPG	5.8	0.0	5.8	5.8	4.3	0.0
PLATPG	7.6	0.1	7.6	7.6	5.7	0.0
PG	13.3	0.1	13.3	13.3	10.0	0.0
LSRRG	0.0	0.0	0.0	0.0	6.3	9.5
PLATRG	0.0	0.0	0.0	0.0	3.4	5.2
HSRRG	0.0	0.0	0.0	0.0	0.2	0.3
RG	0.0	0.0	0.0	0.0	10.0	15.0
Objective function	-7.24E+04	5.93E-13	-1.26E+05	-2.45E+05	3.23E+05	-1.85E+05

VI.2.4. Discussion of Results

Case # 1: This was the base case with a \$2 difference between diesel and RG, \$5 between diesel and PG, and \$2.3 between light and heavy feeds with the environmental penalty. The simulation was run, and a base case was established with an objective function value of $-7.24E+04$. Price differentials were taken based on old prices, which are especially noticeable during the summer mode. The differential between some white products and crude oil was high, since some extra costs were included in the prices, simulating the price of products if they are to be imported.

The model suggested charging only cheap heavy crude and producing about 13 KBPD of PG. It is the maximum blendable PG, whose constraining specification was the octane number, RON. If the RON was relaxed, then more PG or even RG can be produced. The model easily met the RVP specification. The RVP of the PG was 9.4 and the limit was 12.7 PSI. An interesting point noted was that the RVP of the LSR was 18.4, which indicated that it was not stabilized—i.e., it contained a good deal of light ends).

Case # 2: In this case, the heavy crude was penalized an additional \$1.0, increasing the total penalty to \$3.0, which made it not very attractive to operate. The refinery ran only 1 KBPD or 1% of its capacity, which with the tolerance level could be assumed to be zero. The objective function was positive; that is, a negative margin or loss. The program tried to use some of the light crude to minimize the losses, but still the economics did not suggest continued operation.

Case # 3: This was the same as the base case, but the PG was rewarded another \$4. This was the case in the summer mode, when there is a lot of demand for PG. The economics in this case were better than the base case, with objective function value = $-1.26E+05$ or a little less than double that of the base case. The process conditions were the same as those of the base case since some of the capacity constraints were changed.

Case # 4: This case was same as the base case but the prices of all the "white products" were the same. White products are all crude fractions except heavy oil such as reduced crude. In this case, white products included PG, RG and DSL. Thus, diesel and regular gasoline were over-rewarded. This may be the case in some countries due to circumstances that require the refiner to give equal importance to all "white products," especially if supplies from international markets take a long time to reach the target area. It is also sometimes the case for diesel when its price exceeds the price of premium gasoline. However, in our study the objective function improved, reflecting the higher sensitivities to prices.

Case # 5: In this case, minimum production constraints of 10 KBPD were imposed on all white products (PG, RG and DSL). The model had to meet the demand by switching to expensive light crude, which is capable of meeting the additional 7 KBPD demand for gasoline. The objective function value was

3.23E+05, indicating losses. This is good since it represents the situation of many refineries where domestic fuel needs rather than profit is the primary goal.

Case # 6: This was the same as Case # 5 but with relaxed diesel and lower RG limits. This changed the product slate completely. First, a composite blend of 16 % light and 84 % heavy crude was selected to meet the demand for the RG of 15 KBPD. No PG was suggested. This is the case in countries where many low performance cars are used that do not require high RON. In this study, the objective function value improved sharply to -1.85E+05.

VI.2.5. Conclusion

These cases illustrate the effect of capacity constraints, prices, process limitations, and supply and demand effects. Other advanced variables such as effect of reactor temperature on RON and related economics were not covered. The environmental constraints of detailed streams were also not covered; instead, all of them were combined as sulfur penalty in the crude. In actuality, this is the case, for example, for the carbon tax, which penalizes the entire crude barrel for its carbon content rather than penalizing for final product compositions or actual emissions. Thus, from a global corporation point of view, this approach may be more practical in deciding the best feed for long-term products supplies.

VI.2.6. Nonlinear Programming Results

The same problem was solved on a nonlinear programming platform using PIMS. As mentioned earlier, the nonlinear algorithm is based on successive linear programming. The results were considerably improved over those for straight linear programming. Case # 5, which showed a significant loss under linear programming, showed a small positive margin under nonlinear optimization. However, this depends on the degree of nonlinearity of the problem and constraints. In some cases, the optimal solution lies under the convex region, which the linear optimization cannot reach. Figure VI-1 shows a comparison between linear programming results simulated on MATLAB and successive linear programming results simulated on PIMS. It also shows the benefits of implementing a nonlinear solver, especially when the optimization problem becomes tighter.

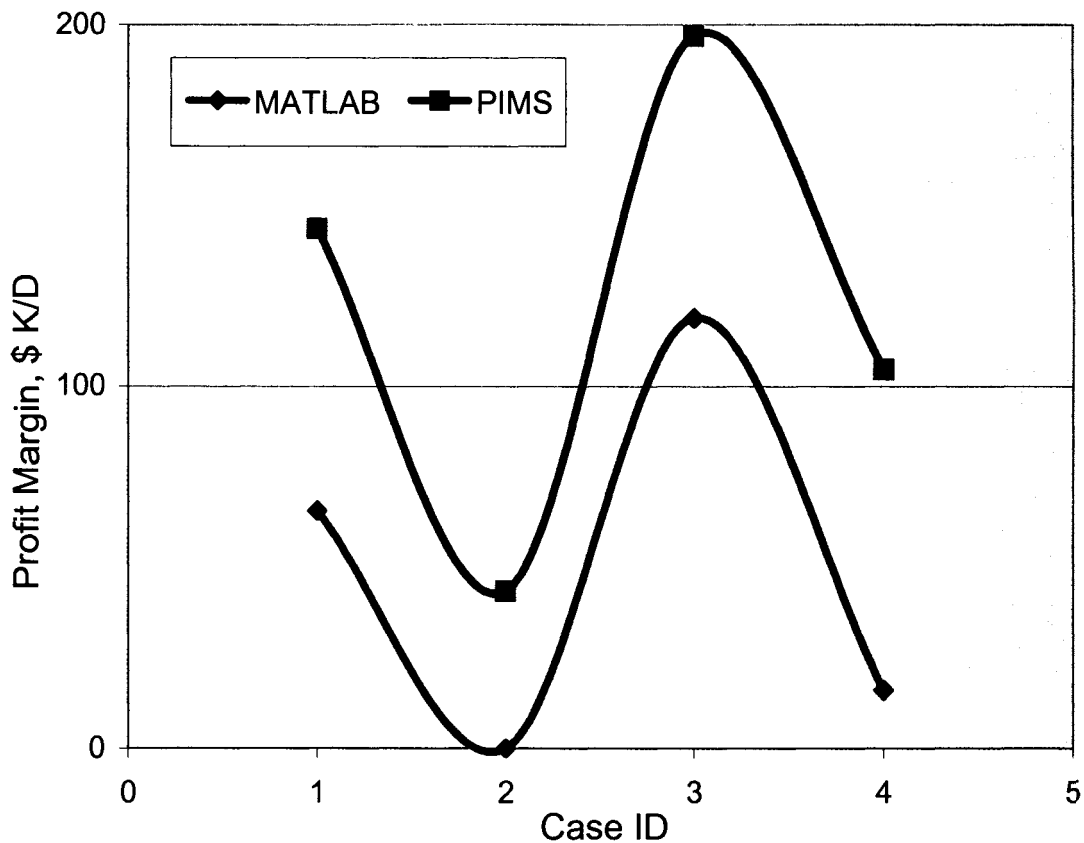


Figure VI-1: A Comparison Between MATLAB and PIMS Results Shows the Benefits of Implementing SLP

VI.3. CATASTROPHIC FAILURE EFFECTS OBJECTIVES

In addition to the cases mentioned above, various scenarios for catastrophic failure were developed to simulate the consequences of catastrophic events on products' supply and profit margins. In all cases, minimum requirements were imposed on diesel as being the most important fuel for transportation and power,

especially in the event of war. However, at this point it was assumed that the model did not include a distillate Hydrotreater.

Various scenarios were carried out on the crude unit to simulate its working at 50, 60, 75 and 100% capacity. Normally, the minimum turn-down for a crude unit is 60 %. With a crude unit of 100 KBPD, it was assumed to have four different crude trains, and the simulation was carried to determine whether one or more of these trains would be completely affected. In addition, the 60 % case can represent partial damage, where the unit is able to run at the minimum turn-down ratio while giving good fractionation. The 50 % case is the worst-case scenario in which two trains are completely down, but the unit may still operate to feed downstream units.

These cases were simulated using mixed integer programming or more specifically binary variables for each crude train. Hence, for the crude unit having four crude trains, one has the following:

$$CH = \sum \text{feed } j \cdot Tr_j, \quad Tr_j \in [0,1] \text{ binary} \quad \text{VI-1}$$

$$= \text{feed }_1 \cdot Tr_1 + \text{feed }_2 \cdot Tr_2 + \text{feed }_3 \cdot Tr_3 + \text{feed }_4 \cdot Tr_4. \quad \text{VI-2}$$

Typically, the feed for each of the trains is equal. Thus, for the crude unit having a total capacity of 100 KBPD, each of the four trains has a capacity of 25 KBPD, assuming that the fouling of exchangers and other process conditions are equal for each train, which is a reasonable assumption. These trains were simulated to have a binary operation—that is, they either shut down or operate while

having the ability to run at full capacity, even though the optimum operation may require running at less than the maximum throughput. Thus, the values of Tr_j are typically 0 or 1, where 0 indicates that the train is not in operation and 1 indicates it is in operation.

For the case of the crude unit running at 75 % capacity with train # 4 shut-down, this is equal to :

$$CH = 1000 * (25 * 1 + 25 * 1 + 25 * 1 + 25 * 0) = 1000 * 75 = 75 \text{ KBPD.}$$

Similarly, the reformer had two trains, which is typical for this size. Cases were simulated for 50, 75 and 100 % capacities. The 50 % capacity indicates that one train is shut down completely; whereas, 100 % operation requires both trains to be fully functional. However, the 75 % capacity simulates a case in which the unit itself may be operable but limitations may occur from other process constraints or equipment due to the catastrophic failure. This may be a compressor problem, coking in some process equipment, indicating a crash shut-down and possible heat surge, or a capacity constraint in the naphtha Hydrotreater.

It is known that a reverse relationship exists between the reformer throughput and gasoline octane, and yield due to higher space velocity. However, the Reformate RON was kept constant at 104, which is at the high end and will not increase much by decreasing throughput. Instead, a more reasonable

gasoline yield increase was assumed with the decrease in the feed rate. An alternative supply of high-octane gasoline was not offered.

It was assumed that utility cost would not change much due to catastrophic events, and it was therefore lumped into the category of intermediate product costs and unit operating costs. Usually a nonlinear relationship exists between the utility cost and the unit throughput, but since this is a small portion of the total economic picture, the relationship may be assumed to be linear and may even be ignored when comparing two different processing scenarios.

VI.3.1. Results and Conclusion

Conditions and results for each of the simulation cases are summarized in Table VI-4. Key factors from this table are graphed below. Since the product supply could not be met with the decreased refinery crude and reformer capacities, it was necessary to import low sulfur diesel to meet the demand. However, the gasoline requirement was relaxed, but this led to extreme cases in which excess naphtha had to be exported to continue operations.

Table VI-4: Catastrophic Failure Results

	1	2	3	4	5	6	7	8	9	10
base case	OPT	OPT	OPT	OPT	OPT	OPT	OPT	OPT	OPT	OPT
Solution Status:	OPT	OPT	OPT	OPT	OPT	OPT	OPT	OPT	OPT	OPT
Case No:	1	2	3	4	5	6	7	8	9	10
Crude capacity, %	100.0	75.0	60.0	50.0	100.0	100.0	75.0	75.0	50.0	50.0
Reformer capacity, %	100.0	100.0	100.0	100.0	75.0	50.0	75.0	50.0	75.0	50.0
Profit Margin, \$ K/D	143.4	107.6	32.1	-18.3	143.4	143.4	113.5	116.5	-14.3	-14.3
FEEDSTOCK PURCHASES										
Arab Light										
Arab heavy	100.0	75.0	60.0	50.0	100.0	100.0	75.0	75.0	50.0	50.0
LOW SULFUR DIESEL										
PRODUCT SALES										
Unleaded Premium	13.3	10.0	8.0	6.7	13.3	13.3	10.2	10.2	6.8	6.8
Regular gasoline										
Diesel	40.0	30.0	30.0	30.0	40.0	40.0	30.0	30.0	30.0	30.0
Fuel Oil	45.0	33.8	27.0	22.5	45.0	45.0	33.8	33.8	22.5	22.5
CAPACITY UTILIZATION										
Crude Unit	100.0	75.0	60.0	50.0	100.0	100.0	75.0	75.0	50.0	50.0
Vacuum Unit	45.0	33.8	27.0	22.5	45.0	45.0	33.8	33.8	22.5	22.5
Reformer	9.2	6.9	5.5	4.6	9.2	9.2	6.9	6.8	4.6	4.6
ECONOMIC SUMMARY ANALYSIS										
GROSS MARGIN	143.4	107.6	32.1	-18.3	143.4	143.4	113.5	116.5	-14.3	-14.3

The objective function dropped from + \$143.4 K/ day for the full capacity to -\$18.3 K/Day for 50 % crude capacity. Note that in this case the positive objective function indicates the profit. Figure VI-2 shows the combined effects of the drop in crude capacity and reformer output on the profit margin, as it reflects the cost required to meet the demand by rerouting feeds or importing finished products.

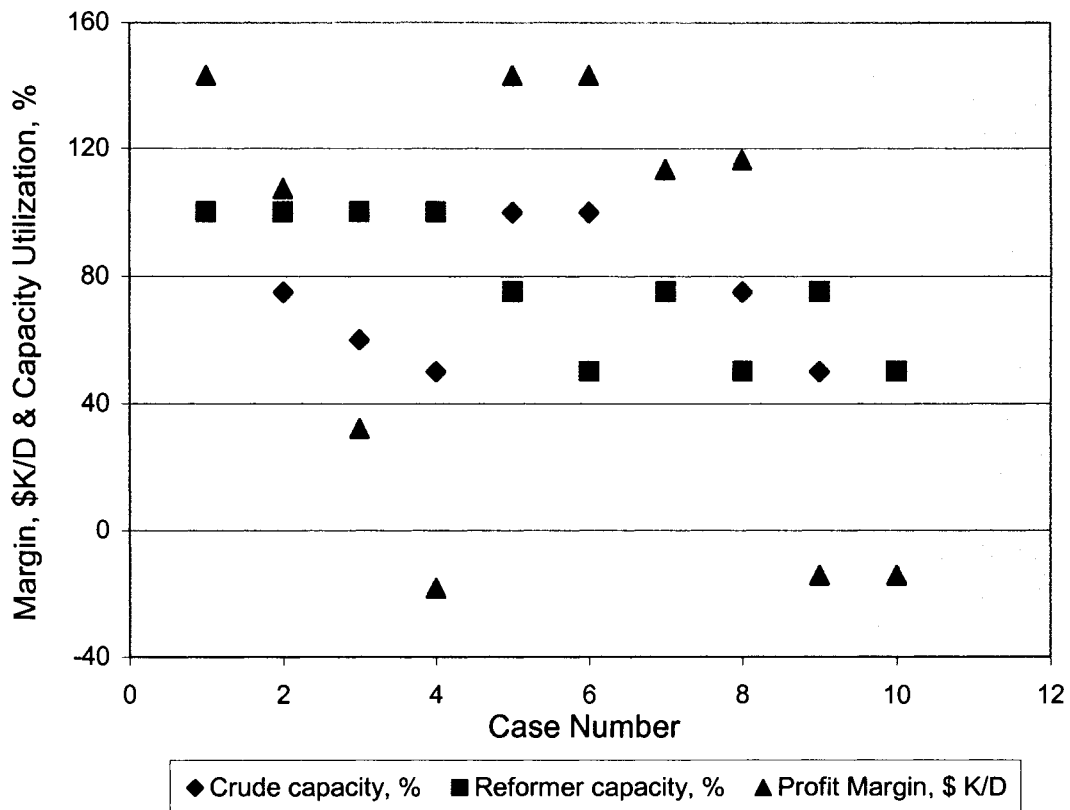


Figure VI-2: Capacity Effect on Profit Margin

Surprisingly, reformer utilization did not affect the objective function much because of the high reformer RON and increased Reformate yield with decreasing reformer throughput, which helped in compromising the gasoline blending specification. Figure VI-3 shows effects of crude capacity on profit margin.

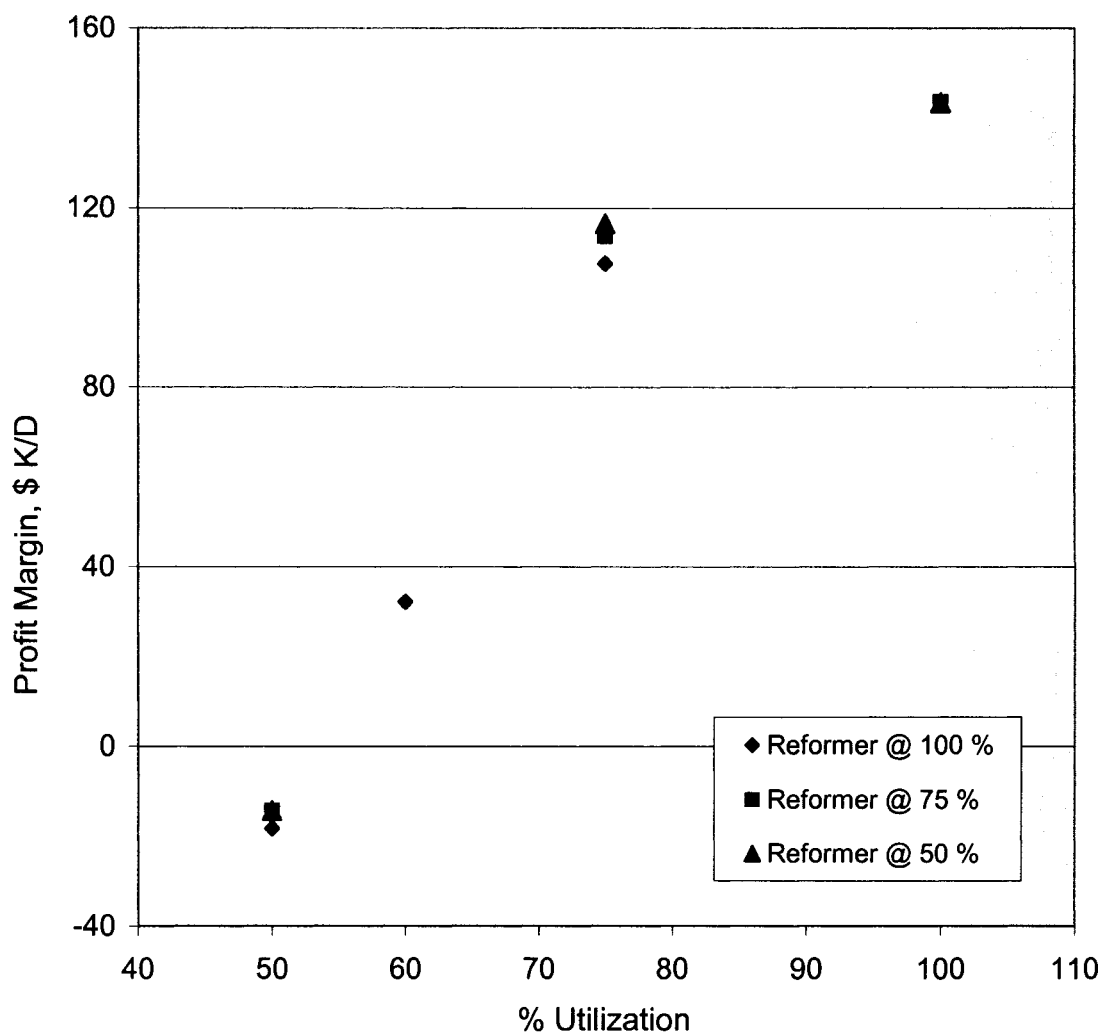


Figure VI-3: Effect of Crude Capacity Utilization on Profit Margin at Constant Reformer Output

In addition, several cases were studied to examine the effects of product specifications on the overall refinery optimization model and product allocation.

Diesel sulfur content was taken as an example. Usually diesel sulfur specifications act as a constraint on many refineries, and diesel cannot be Merox-treated (a process converting sulfur from a harmful to a non-harmful form without desulfurizing the hydrocarbon product). However, gasoline and jet fuels can usually be Merox-treated without need of desulfurization. High sulfur fuel oil can also be sold in the open market for use as a bunker fuel or for power plants. This is a challenge facing many developing countries that want to enhance their fuel specifications but do not have enough capital to build expensive hydrotreating facilities. For cases of catastrophic failure affecting the supply/demand chain or the ability of a refinery to produce diesel at the required low sulfur specifications, an alternative for gradually relaxing diesel specifications was studied to determine how a refinery can meet the local demand for diesel under such circumstances. Figure VI-4 shows effects of diesel sulfur on profit margin.

A choice of importing 500 PPM sulfur diesel from international markets was given a higher price. In addition, a maximum import limit was imposed to simulate logistics constraints. The effect on the objective function was nonlinear, but it reached a maximum value corresponding to the diesel specifications being inactive; that is, the amount of diesel coming out of the crude unit without treatment met the temporarily relaxed new sulfur specifications which may be necessary the event of war or other catastrophic events. The model needed to import low sulfur diesel, LSD, to meet the demand, which was preset at 30 KBPD. At the extreme limit of 500 PPM sulfur, the model did not converge due to its unfeasibility.

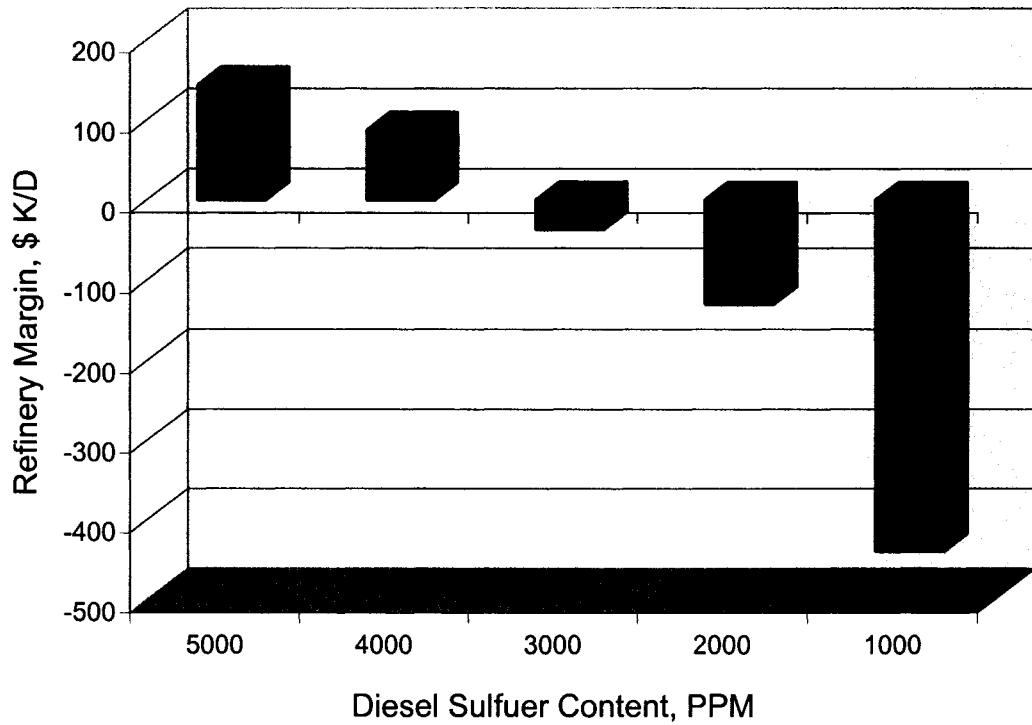


Figure VI-4: Effects of Diesel Sulfur Content Specifications on a Refinery's Margin

VI.4. MULTI OBJECTIVE-SINGLE REFINERY OPTIMIZATION

CONCLUSION

This chapter has laid the foundations for optimizing a refining system consisting of multi refineries, multi markets, different specifications, different product tiers, and different seasonal requirements. In addition, the profit (or cost) function has the capability of including the multiple objectives embedded in it after being quantified to monetary terms, which makes it easier for decision-makers to

select the optimum operating scenario for the refining system under rapidly-changing crude prices and world political conditions.

For this section, case studies were carried out on multi market, multi objective within a single refinery system. The following chapter will expand the work to cover multiple refineries to determine if it is better to have refineries specialized in certain products or to pay more in order to have the flexibility of meeting the demand in the event of a catastrophic failure, whether the advantages justify the cost, and to address the alternatives and the degree to which they can fulfill demand requirements.

The present chapter has shown the importance of crude capacity on refinery profitability even in the absence of sufficient conversion capacity, if straight-run product prices are sufficiently high to ensure positive topping or hydroskimming margins. It has also shown the exponential growth in cost to meet specifications in the absence of sufficient treating capacity as product specification constraints become more stringent.

VII MULTI REFINERY CASES: CATASTROPHIC FAILURE EFFECT OBJECTIVES

Different scenarios were set up to simulate the consequences of catastrophic events on product supply and profit margin. Different refineries were assigned different scenarios depending on the location, proximity to oil supply channels (such as seaports or pipelines), the complexity factor of the refinery (which relates to the presence of treating and conversion units), and availability of alternatives. All of the cases presented here are based on actual refinery situations, with some figures and constraints modified for confidentiality purposes.

VII.1. CASES

VII.1.1. Increased Risk from Targeting Crude Oil Tankers Supplying a Refinery with a High Turndown Ratio but Single Feed Source

In this case, the aim was to simulate the increased risk of targeting crude oil supplies at a refinery with a high turndown ratio but single feed source—that is, vessels (ship crude carriers). The simulation began with Refinery # 3, which

is a small refinery having several crude units and relatively far from tension zones. The main constraint for this refinery was crude supply since it receives crude oil through vessels that can be targeted. A penalty for the increased risk (such as insurance cost or delay in delivery) was gradually added to the objective function and embedded in the crude cost. Another constraint was that this refinery can only process light crudes in the range of 32-35 API due both to the limitations of the crude units' overhead condensers and the internal design of the distillation tower. Cooling problems are serious issues in countries in the Middle East, especially during summer, when they can limit not only the fractionator's output but the entire refinery's throughput.

VII.1.2. Increased Risk from Targeting Crude Oil Pipelines Supplying a Refinery with a Single Feed Source

This case was simulated for Refinery # 4, which is a large topping facility with only one source of feed and the ability to process only light crudes. The refinery is supplied with crude through a portion of pipeline that is connected to a main header feeding several other refineries. Increased penalties were imposed on the transfer cost of the portion of the pipeline feeding only this refinery, even though other refineries share the main pipeline header. This simulates the case of damage to the portion of the pipeline feeding only this refinery. In this case, it was assumed that crude was transferred by pipeline to an oil terminal and from there it was distributed to other refineries either by pipelines or by small tankers.

VII.1.3. Total and Partial Capacity Losses as a Result of a Catastrophic Failure

These cases were simulated for Refinery # 1, which is a large facility having the capability of processing different crudes and condensate. This refinery is considered as the workhorse of the supply of distillate and jet fuels which is particularly important during wartime. [However, the turndown ratio for this refinery is lower than other refineries since it is a modern refinery built after 1980, when economics favored having a single large crude fractionator]. Later, another condensate splitter was added. Even though this configuration results in very low operating costs, and much lower parts inventory and maintenance problems for the refinery, it does not offer much flexibility in processing different crude types simultaneously or having low turndown ratios. Note that the products from each refinery are derived from the following equation:

$$\text{Product } i = \sum \text{Product }_{ij} \text{Tr}_k, \quad \text{Tr}_k \in [0,1] \text{ binary} \quad \text{VI-3}$$

$$= \text{Product }_{i1} \cdot (0 \text{ or } 1) + \text{Product }_{i2} \cdot (0 \text{ or } 1) +$$

$$\dots \text{Product }_{in} \cdot (0 \text{ or } 1) , \quad \text{VI-4}$$

where

- The product is any petroleum product such as low sulfur diesel, JET-A1, etc.
- i is the product number.
- J stands for the refinery number.

- Tr_k stands for the unit or train abbreviation, and k is a binary variable to show that the selected unit or train in a unit is either on or off.

Three scenarios were carried out for this refinery:

1. Partial loss in the condensate splitting capacity, which could be due to one or more of the following possible reasons:
 - a. Logistics of supplying the refinery with condensate, such as an attack on the pipeline or constraints on the flow due to pumping limitations as the result of an attack, mechanical failure or cooling limitations.
 - b. Loss of processing capacity in the condensate splitter column, products coolers, overhead condenser or downstream product treatment of the condensate section of the refinery.
2. Total loss of condensate capacity together with decrease of crude capacity to the minimum running capacity. This could be the result of a partial outage in the crude unit, such as loss of one or more crude trains.
3. Hydrocracker unit flexibility loss. In this scenario, no constraint was imposed on the refinery capacity, but a constraint was imposed on the Hydrocracker unit, decreasing its ability to run in diesel mode. This is important in producing high quality distillates and is needed not only for the production of diesel but also for blending with straight-run high sulfur diesel from the crude unit to make it salable. A loss in the hydrocracked diesel of 5 KBPD may cause more than double this amount of loss in the total diesel available for sale. In

addition, very low sulfur diesels are usually produced from hydrocrackers, and this constraint can affect the supply of low sulfur diesel to the whole country, as will be discussed in the results.

VII.2. RESULTS

For the first case of Refinery # 3, the refinery gradually had to drop production due to the imposed penalty. However, minimum production had to be maintained in order to meet demands that had been assigned to this particular refinery and could not be switched to other refineries.

For Refinery # 3, an interesting result was obtained namely, that the local objectives of the refinery increased with increasing oil prices until the crude price reached \$26/BBL, after which it decreased. However, the global objective decreased as the crude prices increased. This is shown in Figure VII-1. The local optimum for this refinery is clearly not the global optimum, and the refinery demonstrates a strange phenomenon in the objective with increasing feed prices. This is due to the complicated pricing structure for this particular refinery, since it makes money by selling intermediate products to a nearby lube refinery and the prices of these intermediate products are based on crude prices. Consequently, an increase in crude prices will cause a temporary increase in the price of intermediate heavy fuels sold to the lube refinery but only up to a certain point. After that point, the effect of the increasing crude prices will affect the economics of the refinery, since most of the crude is consumed by the refinery itself.

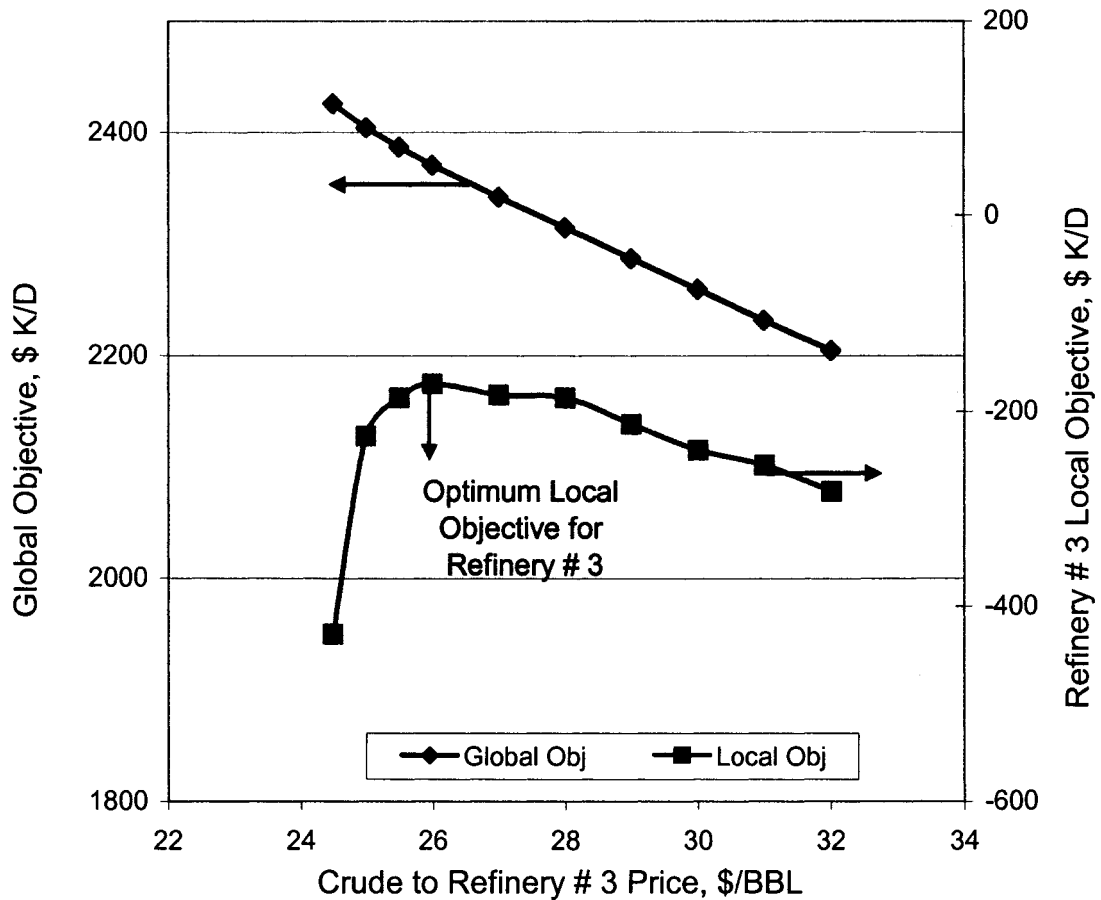


Figure VII-1: Effects of Increased Crude Price (Due to Increased Risk) on Local and Global Objectives

For Refinery # 4, the results demonstrated that the local objective did not match the global objective but was mainly a function of the refinery’s capacity. This is another example of the nonlinear relationship between both objectives, as can be seen in Figure VII-2. This figure also shows that the penalties did not affect the refinery’s capacity in a continuous but rather in a discrete manner.

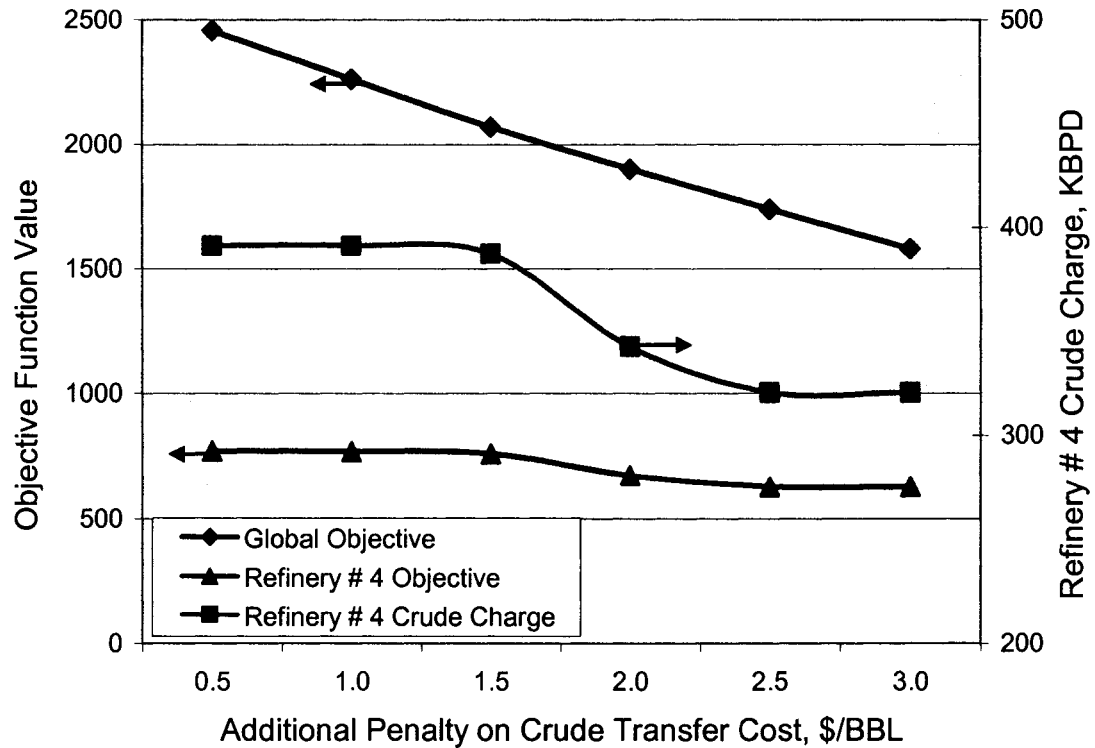


Figure VII-2: Effect of Transportation Cost Penalties on Capacities and Objectives

For Refinery # 1, the local and global objectives were more correlated than those of the other two refineries for all scenarios, as shown in Figure VII-3. This is due to the large size of the refinery, which comprises about one-third of the total refining capacity of the country.

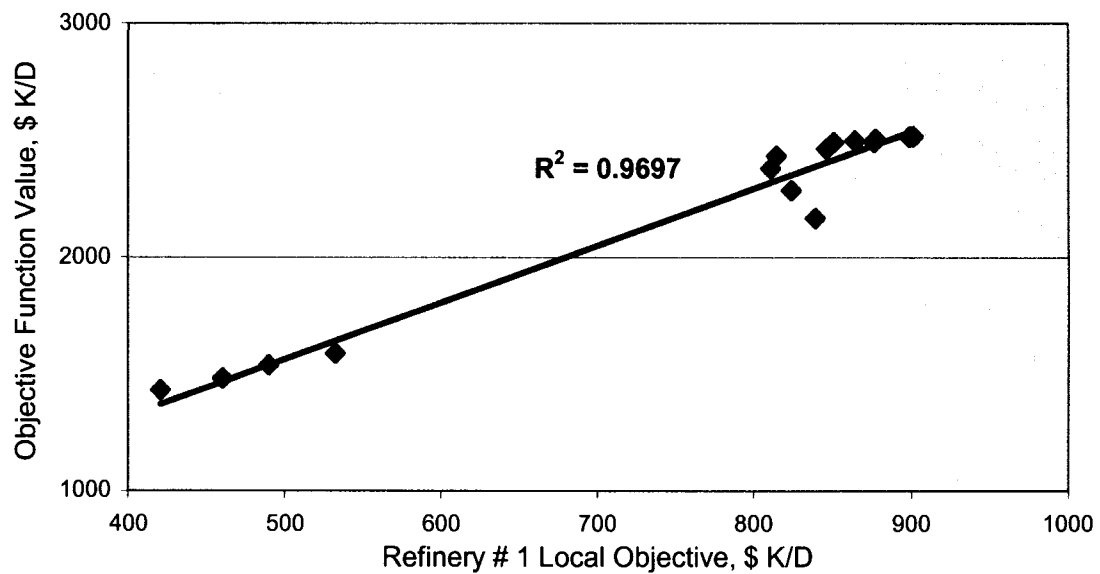


Figure VII-3: Relationship between Global and Refinery # 1 Objectives for All Cases

Figure VII-4 shows the effects of condensate capacity loss on margins and products yields for different products in scenario # 1. This is due to the availability of alternatives and the composition of the condensate. This effect was most noticeable on the production of unleaded gasoline (regular). The second product was low sulfur diesel. In both cases, the effect was mainly observed after the capacity loss exceeded 40 %.

For scenario # 2, the results showed that the effect was clearer on the objective function for both local and global objectives. Figure VII-5 shows the relationship between the condensate processing capacity and selected light products yields.

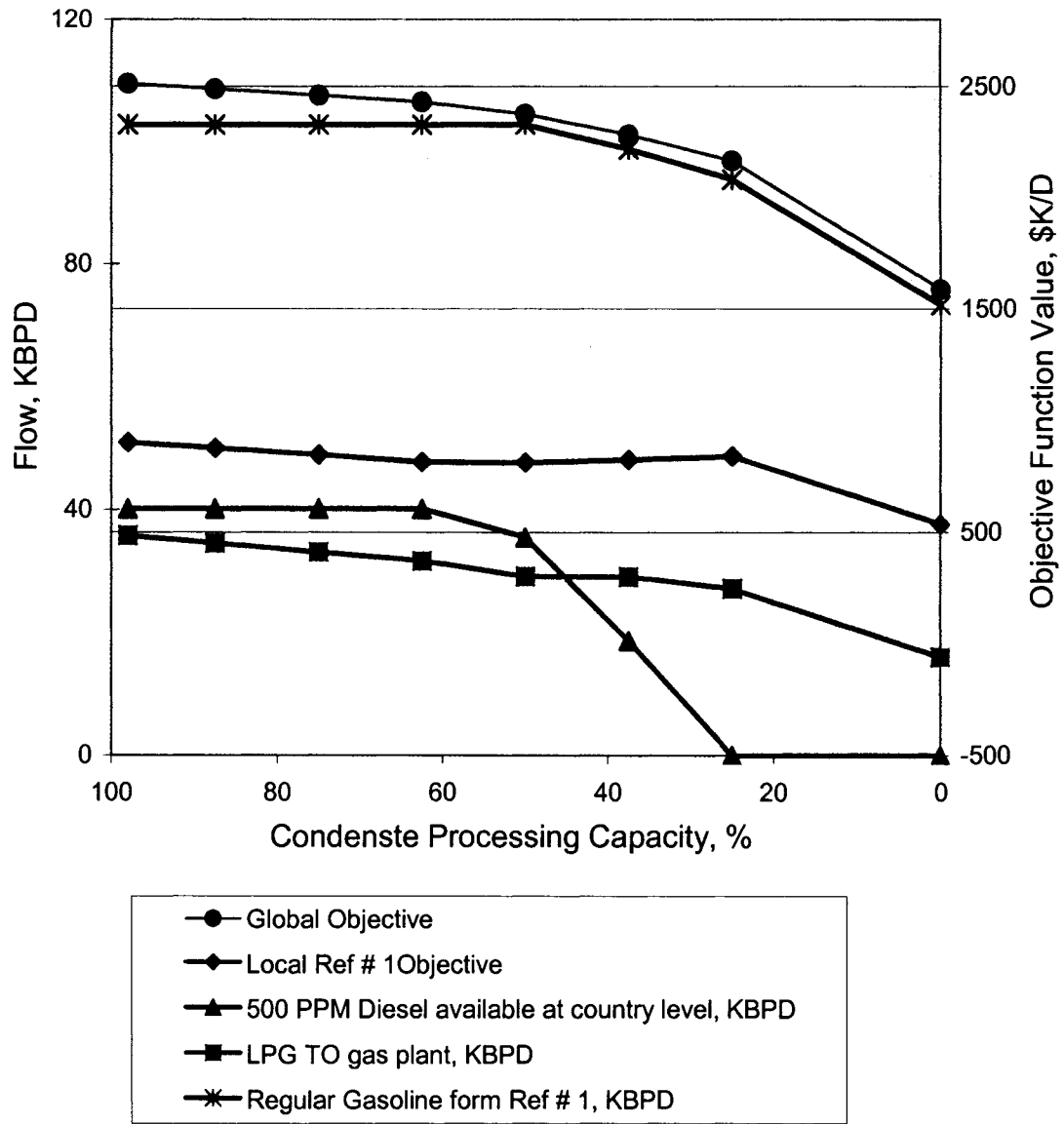


Figure VII-4: Effect of Condensate Capacity Loss on Objectives and Products Flow

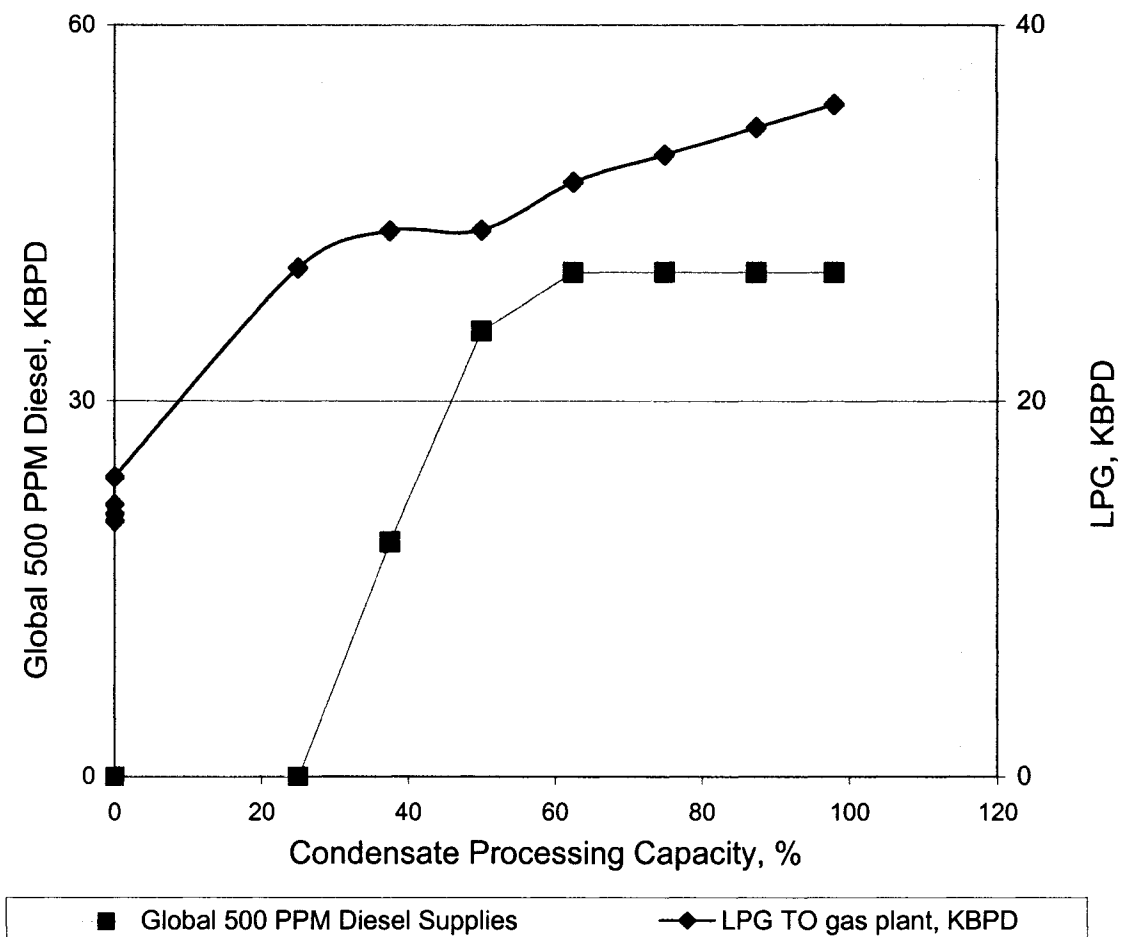


Figure VII-5: Effects of Condensate Processing Capacity Loss Together with Partial Loss in Crude Capacity on Selected Light Products

Scenario # 3 yielded some interesting results, as shown in Figure VII-6 namely, that both global and local objectives were not significantly affected by the loss of 50 % of Hydrocracker flexibility, even though this had a significant effect on the refinery's overall low sulfur diesel (LSD) production. This is mainly due to the fact that the total Hydrocracker output is not affected; rather, it is the quality and composition of products that are affected. That is, the Hydrocracker

charge in all cases is about 100 % of the base case, but due to limitations on the diesel mode capacity, the unit cannot run toward maximum distillate but can rather go to the maximum constrained limit and reach a point between maximum naphtha and maximum distillate modes. The main issue is that the amount of LSD available to the country is critically affected, even though it does not appear to affect either the local or the global objective functions.

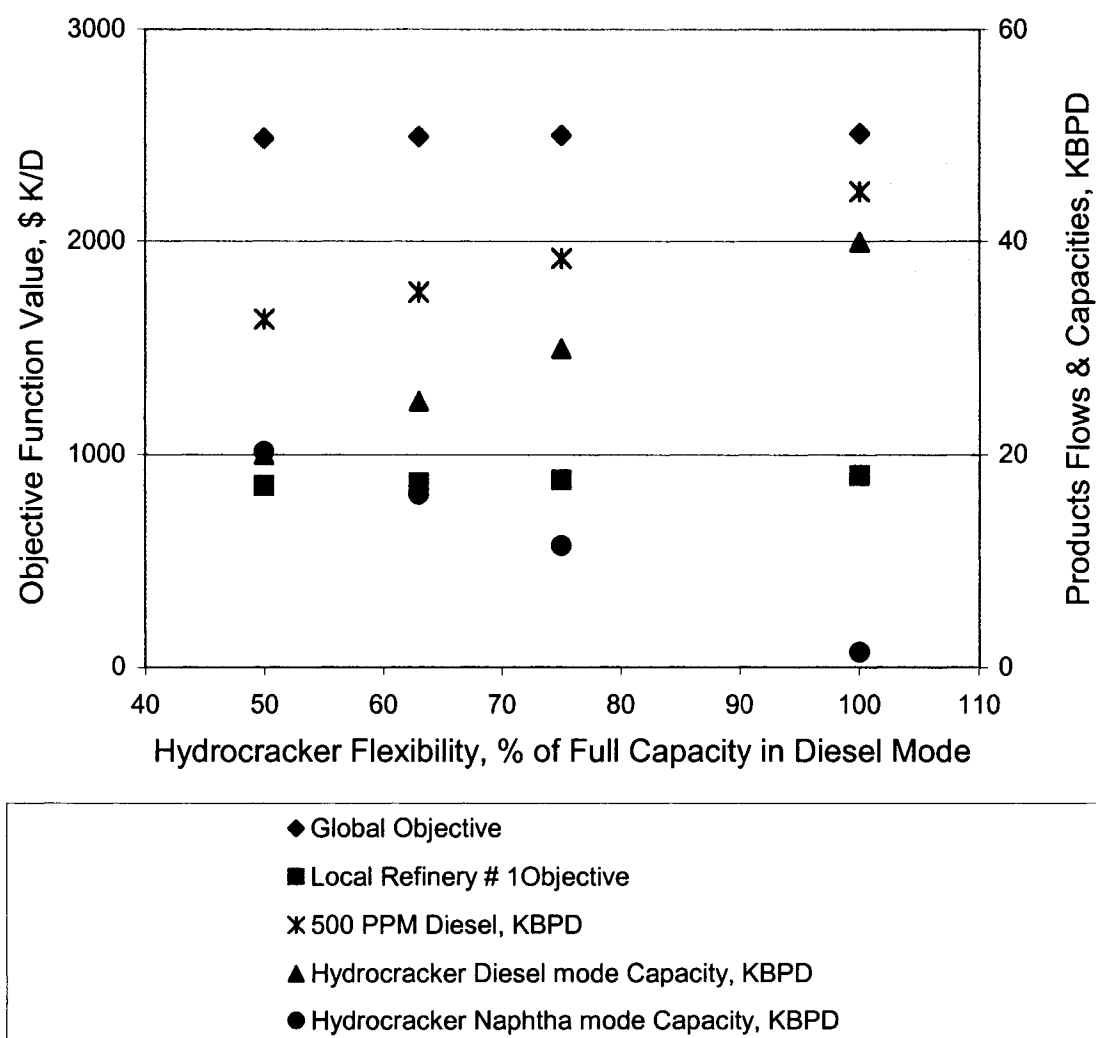


Figure VII-6: Effect of Hydrocracker Flexibility Loss on Objectives and Capacities

VII.3. CATASTROPHIC FAILURE EFFECTS OBJECTIVE

CONCLUSION

1. The results demonstrate that refineries can have a local multi objective optimum that does not follow the same trend as either the global objective or the local single objective optimum (discussed below).
2. In addition, the results indicate that the relationship between the global and local optimum may not always be linear. Moreover, the two objectives may not necessarily move in the same direction or at the same rate. This is a factor related to the internal complexities of refineries and the types of imposed constraints.
3. For refineries, the multi objective local optimum may be different from the local optimum with regard to economic objectives. The deviation from the economic optimum depends on the degree of flexibility of the refinery both in selecting different feed/product schemes and in having different operating modes. These flexibilities act as a relief from imposed multi objective constraints by providing more alternatives to the model, which increases the feasible region and thus leads to a more optimal solution. Transportation costs of feeds and other intermediate products are also significant factors.
4. For most refineries, especially large ones, changes in capacity or in local objectives as a result of imposed constraints usually follow a discrete behavioral pattern in contrast to a global objective, which normally follows a smooth curve. This discrete behavior is due to the fact that refinery op-

erations are hard to change and there are minimum turndown ratios that cannot be exceeded. In addition, the operating cost of a refinery unit is partially fixed. That is, if a unit's capacity is reduced by 20 %, operating expenses such as cooling costs and manpower requirements will not drop by the same percentage. In actual life, changing the operating conditions requires time to stabilize the unit in order to be able to produce on-spec products.

5. For catastrophic failure effects, crude processing capacity is the main factor affecting the objectives. The loss of feed processing capacity such as crude or condensate has more effect on the objectives than the loss of upgrading and treatment capacities such as gasoline reforming. In addition, the results demonstrate the benefit of having more than one crude unit, which gives higher flexibility to run the refinery in less than the 60 % minimum turn-down ratio in case of a catastrophic failure event. That is, for two refineries of the same size, if a refinery has one crude unit, it can usually run at 60 % of the maximum capacity. However, if the same refinery has 'm' crude units, it can run as low as $0.6/m$ of the total capacity.
6. The results demonstrate the importance of examining the effects of loss of internal processing flexibility on product supplies, which may not be clear in either local or global objective functions but will appear at a point at which supplies cannot be met by all the local refineries combined and thus imports are needed. Proper tiers of import penalties should be im-

posed on imports in order to clearly address the shortage of some products in the event of partial or total loss.

7. The price structure of Refinery # 3 creates a conflict between global and local objectives at some points. This is due to the many constraints imposed on the refinery in order to meet the demands of both the nearby lube refinery and the local urban market. The refinery is not sufficiently credited for the imposition of these demand responsibilities, which creates a negative refinery margin. Hence, optimization at the local level may suggest cutting back on most processing operations.

VIII MULTI REFINERY CASES: ENVIRONMENTAL AND PRODUCT SPEC OBJECTIVES

Different scenarios were set-up to simulate the consequences of environmental constraints on product supply and profit margin and to determine whether refineries will be able to conform to the new stringent products specs and at what cost. Another aim was to address, for each product, the optimum levels or regions that provide the greatest reduction in environmentally harmful components with the least impact on both plant capacities and economic objectives.

Different refineries had different scenarios depending on the location, type of products manufactured at the facility, and a market that involves different environmental constraints such as those related to urban and rural areas. All cases presented are based on the situations of actual refineries, with some figures and constraints modified for confidentiality purposes.

VIII.1. CASE STUDIES

VIII.1.1. Effect of Environmental Objectives and Product Specifications on a Specific Refinery-Market System

In this case, the purpose is to examine the effect of environmental objectives presented as product specifications upgrades to a specific refinery-market system. This case is based on an actual situation for an urban market system consisting of north and south bulk plants. The south bulk plant provides products to other cities, as well as to a naval base, a desalination plant and a power plant. Due to design and logistic limitations, some products are only provided to this bulk plant by a nearby refinery, even though some other products are shipped from other refineries to the bulk plant through that refinery.

Considering the consequences of the location of this market, it was assumed that the current medium sulfur diesel having a spec of 4000 PPM sulfur would be upgraded to same low sulfur diesel level of 500 PPM. Even though the new level is high compared to that required in some countries, it is a great achievement, considering that in many developing countries the diesel sulfur spec is 10,000 PPM.

For this case, Refinery # 3 was selected. This refinery, as mentioned earlier, has the limitation of processing only Arab light crude. It also has cooling problems, which are a serious issue in countries of the Middle East especially

during summertime. However, no other refinery in the model produces this type of diesel, even though there are other diesel types which are even lower in sulfur.

Results

The refinery demonstrated a need to import 500 PPM sulfur diesel to be blended with the refinery-produced streams. However, due to logistic reasons, this amount was limited to 10 KBPD. Consequently, with the lowered sulfur content ceiling, the total amount of refinery-made diesel that could be blended became less and less until it reached a point at which continuing at the same refinery output level meant having an unblendable stock of diesel. Some of this diesel was dumped to fuel oil, even though this constituted degradation for diesel and could limit the flash point spec of the fuel oil at some point. This process is clearly shown in Figure VIII-1.

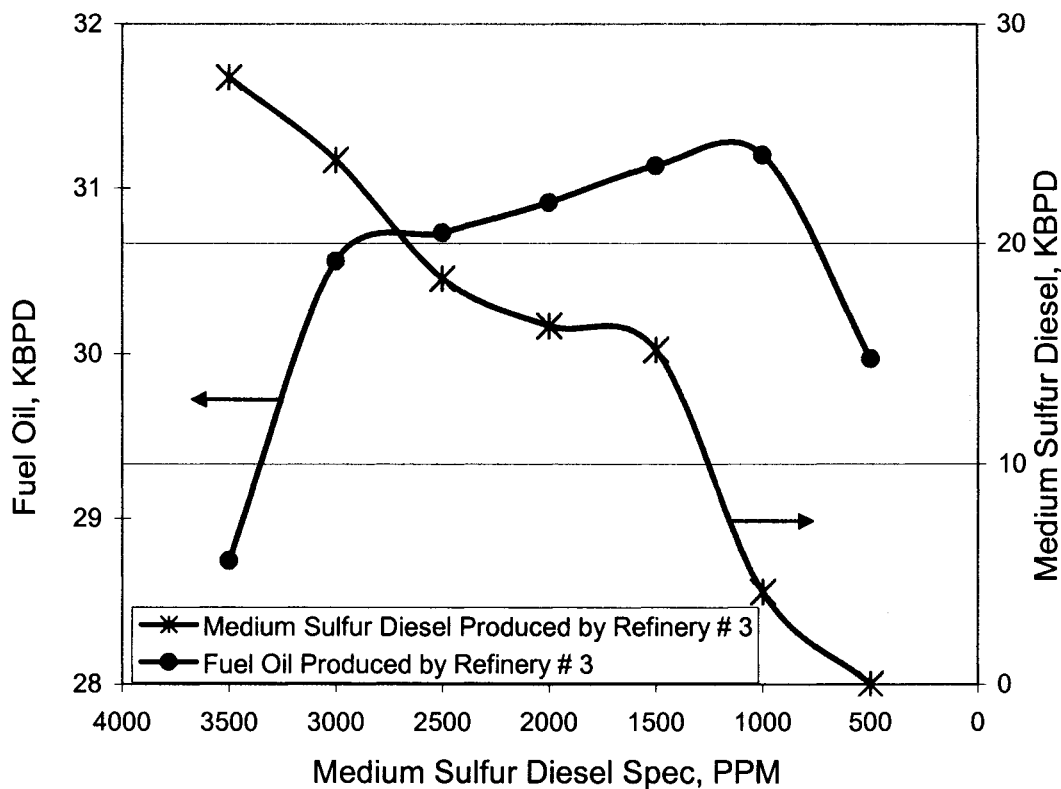


Figure VIII-1: Environmental Objective Effect on a Specific Product-Market System: Un-salable Diesel Being Degraded to Fuel Oil

At this point, the refinery's throughput has to be decreased to avoid having imbalanced product slates, as shown in Figure VIII-2.

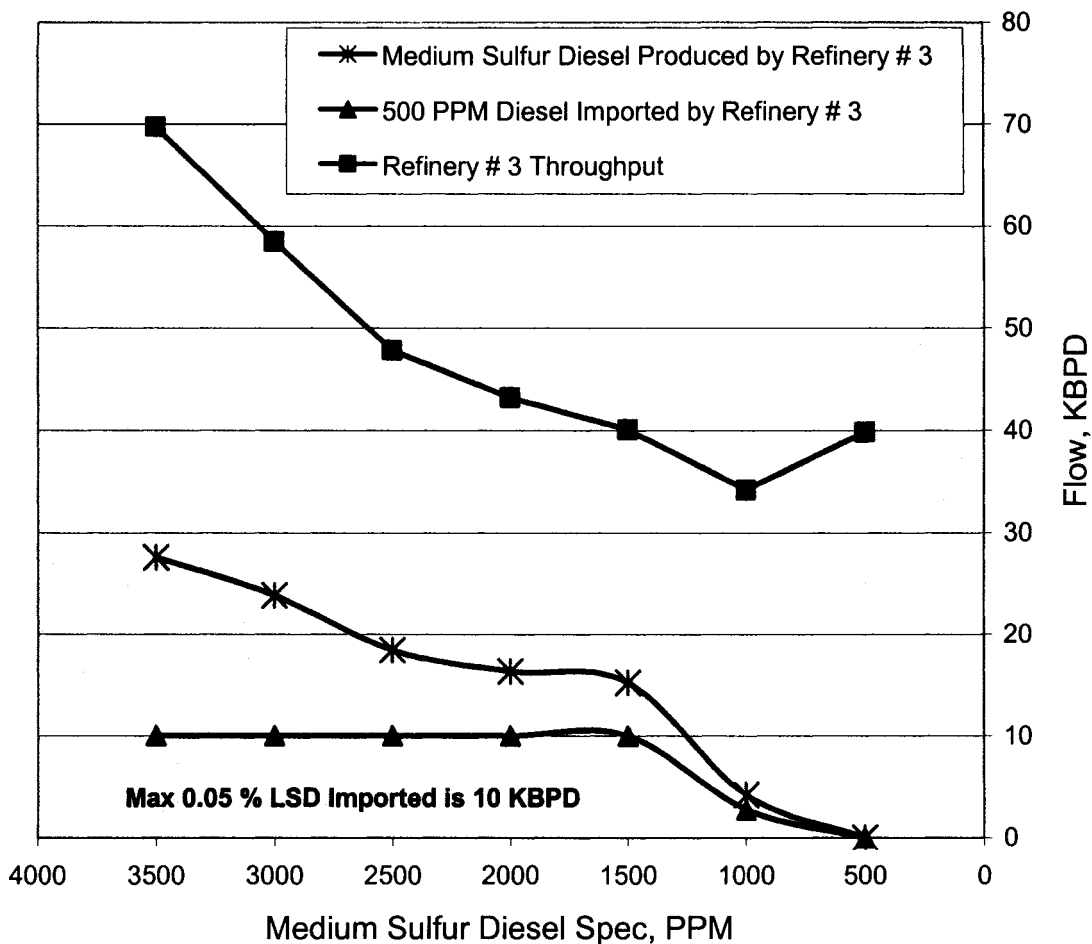


Figure VIII-2: Environmental Objective Effect on a Specific Product-Market System: Unblendable Diesel Limits Refinery's Throughput

This led to interesting results—namely, that the local objective was actually enhanced by the drop in the refinery's throughput. It then decreased at some point following the trend in the global objective. This is shown in Figure VIII-3. Recall that this is the same refinery that always demonstrates such phenomena. This is due to the objective function layout, since this refinery is losing money and has a negative net margin. However, the refinery has to continue in opera-

tion to meet demands. Exerting environmental or catastrophic constraints on the refinery, resulting in a reduction of the refinery's throughput, would decrease its operational losses, while simultaneously weakening the global objective.

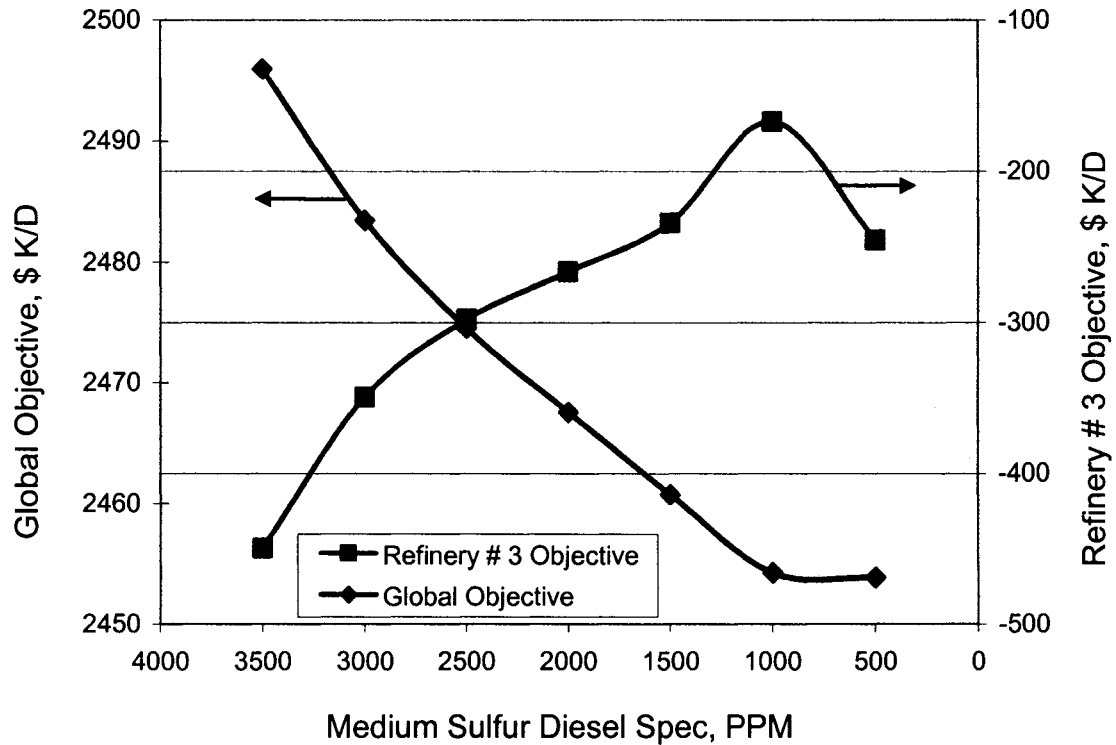


Figure VIII-3: Environmental Objective Effect on a Specific Product-Market System: Inverse Relation between Global Objective and Refinery # 3 Objective

This is a real-life case in many refineries where the objective of the local refinery management is to produce certain products at a profit, while corporate management may visualize a different global production scheme that is believed to be more beneficial on the corporate level but may not satisfy local refineries. The refinery in question reached a point at which it did not make the demand, even after importing very low sulfur diesel to assist in blending with a new spec.

VIII.1.2. Effect of Global Product Spec on the Entire Refinery and Distribution System

In order to examine the effect of environmental objectives and product specs on the entire refining and marketing system, a product available from most refineries and to most of the markets had to be selected. For this case, it was decided to study the upgrade of premium gasoline product research octane number RON specification from the current level of 95 to a new level of 99. The decrease of the RON spec from 95 to 91 was also studied.

Currently, the system we are studying is composed of one grade of gasoline that is available to domestic consumers, even though some refineries can produce different grades of gasoline; however, those products are used either for further blending or for export purposes. The main constraint in having two different grades of gasoline is the distribution and gas station systems, which are currently designed for only one grade of gasoline.

The current gasoline spec is set at 95 RON. This is good for most cars; however, it is too low for some of the best state-of-the-art cars, especially European luxury cars such as BMWs and Porsches. On the other hand, it is higher than what is needed by most cars in local markets, which is about 92 RON. This three degree giveaway in the research octane number can be a substantial loss at the corporate level. Consequently, this study assumed that the entire system could move either way. This was done in order to examine the effect of revising the spec on the system, even though the best solution may be making more than one grade of gasoline available.

Results

All refineries made the new product but at a higher cost and this affected some refineries more than others. Two factors helped in meeting the demand for the new product: the presence of export refineries designed to produce such high RON gasoline by the use of CCR and Alkylation units, and the availability of Methyl Tertiary Butyl Ether (MTBE) as a blending component having a RON of 116. The effect on the global objective was highly linear, as shown in Figure VIII-4.

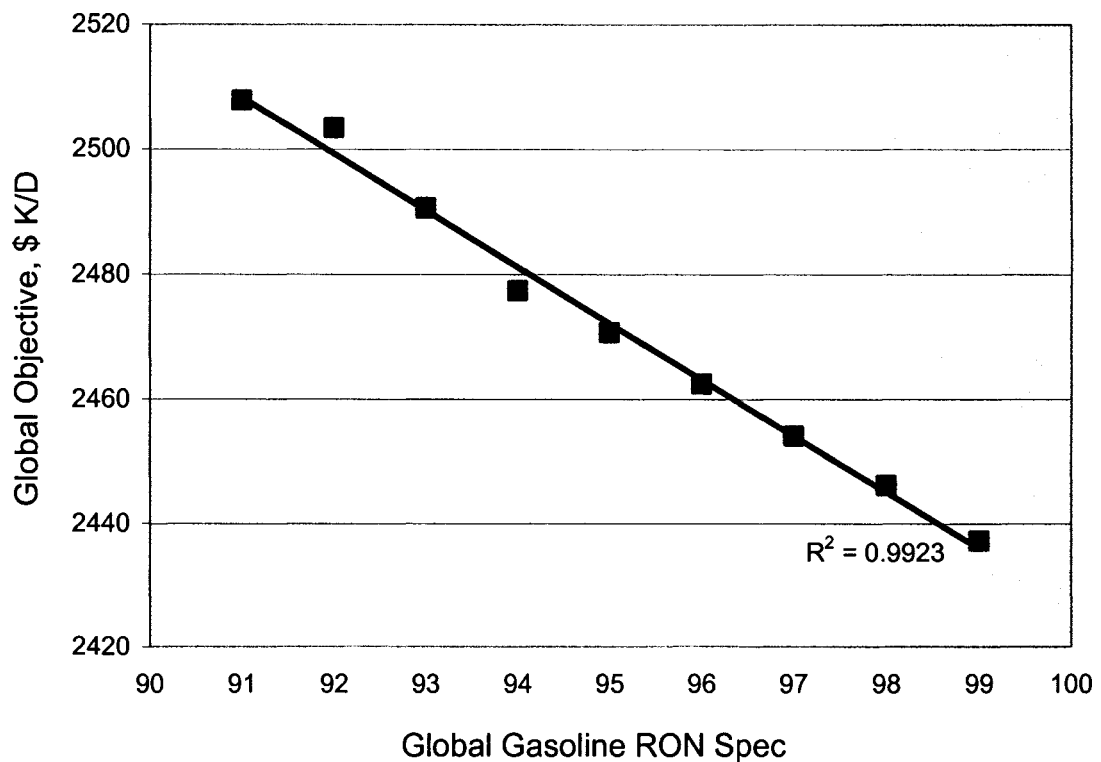


Figure VIII-4: Environmental Objective Effect—Global Gasoline RON Spec: Linear Inverse Relationship between RON and Global Objective

On the other hand, the effect on the local objective of each refinery differed due to the availability of alternatives within the refinery itself and the internal layout of the refinery. Another factor was the cost of shipping if an import from another refinery was needed. This effect differed in relation to various markets or product terminals that obtain different products from different refineries and sell them to bulk plants. For most countries, the prices of petroleum products are fixed by the government, in which case the terminal has to buy products from refineries at differing prices that reflect the actual production cost of the product. However, the terminal may sell products to local bulk plants at prices set by the government, which does not reflect the changes in production costs due to changing product specs. This is shown in Figure VIII-5.

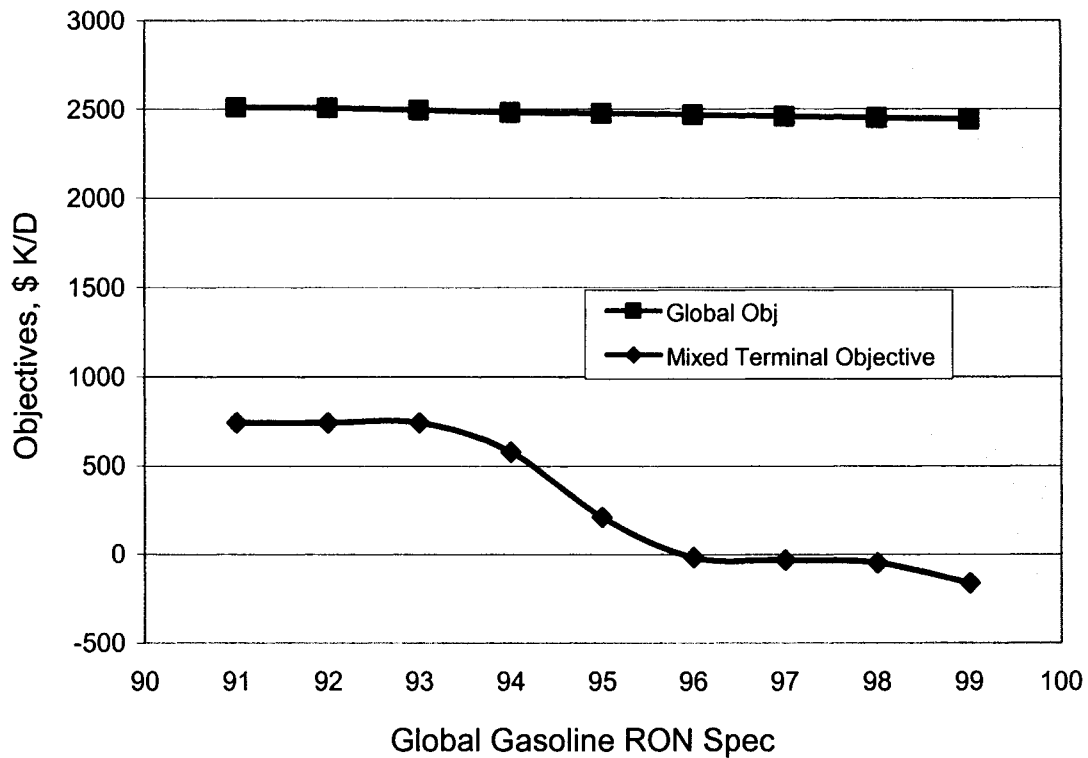


Figure VIII-5: Environmental Objective Effect—Global Gasoline RON Spec: Positive Relationship between Mixed Terminal and Global Objectives

From the simulation runs, it was understood that there is a pseudo-optimum region around 94-96 RON which is the current region of the RON. This may suggest continuing with the same product spec and having one grade of gasoline. However, more study is required to determine the real need for a higher RON market and whether this amount can be met by some but not all refineries or even produced periodically. Note that optimum here refers to the refining system and distribution capability, not to what is optimum from a purely economic point of view. A determination of this would require studying re-pricing the gasoline product at the country level to see if the increase in the price justifies

going beyond the 96 level, or if, on the other hand, the loss in revenue as a result of decreasing the price of low RON gasoline is less than the savings from producing lower grade octane—for example, importing less MTBE. This is an area in which the extended use of advanced nonlinear solvers other than SLP may yield to a better result.

One interesting observation was the inverse relationship between two refineries, as shown in Figure VIII-6. Not by coincidence, the two refineries are in the same geographical area. These refineries are:

1. Export refinery # 1: This is a state-of-the-art export refinery, as mentioned earlier. The refinery is able to produce the most stringent product spec. It can make these products available to other domestic refineries and bulk plants as blending components to help these refineries make their own petroleum products meet the domestic specs.
2. Refinery # 5: This is a domestic refinery that is a simple hydroskimming facility with only a Platformer and a distillate Hydrotreater.

Refinery # 5 imports high quality intermediate blends from export refinery# 1 to use them in blending domestic products to required specs. Thus, any import from export refinery # 1 to refinery # 5 will appear as an increase in export refinery # 1 objective and a decrease in refinery # 5 objective. The amount will not be exactly same due to other costs refinery # 5 has to pay such as product transfer cost. The oscillation in the curves is due to several reasons, some from internal refineries operating costs such as commissioning and decommissioning

for unit, or it can be a result of feed and products quota imposed by the global optimum scheme.

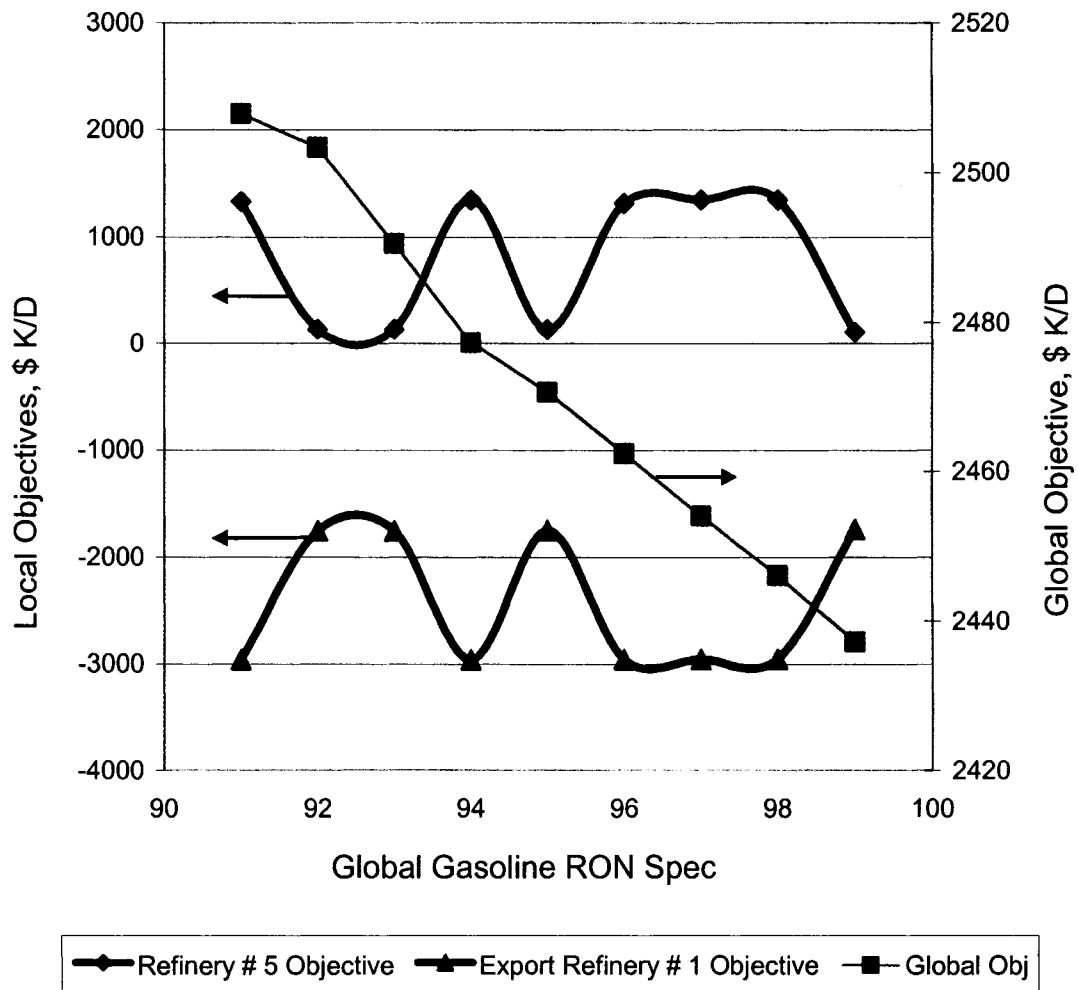


Figure VIII-6: Environmental Objective Effect—Global Gasoline RON Spec: Inverse Relationship between Domestic and Export Refineries

Usually with a conventional fixed bed Platformer, the maximum Reformate RON is set at about 95 to avoid having too frequent regeneration downtime. Increasing the Reformate RON, in other words, increasing severity at the same throughput or liquid hour space velocity LHSV requires higher reactor tempera-

tures, usually over 510° C during the early stages of the cycle. With carbon deposition on the catalyst, higher temperatures are required to produce the same Reformate RON. After a time, either the metallurgical limits of the reactors are approached, or the Reformate yield drops to a level that it becomes better to shut down the unit and carry out catalyst regeneration. This process is termed "cycle life".

In the simulation runs, the objective function coefficients of the refineries at which prices were fixed—that is, those in which we did not change the price of gasoline as its RON changed and in which we did not alter regular gasoline prices--the model was forced to meet the local demand at the same prices for different gasoline specifications. What affects the refineries' margins is the number of intermediate streams needed to produce the required blend, which in some cases must be imported from the export refinery at close to international prices.

VIII.1.3. Environmental Objectives and Product Specs at the Global Level

In this case, it was assumed that the national diesel sulfur spec for low sulfur diesel would change from 0.05% wt, which is 500 PPM to 0.005 % wt or 50 PPM. This is termed severe cutting, which requires deep desulphurization and affects all refineries that produce low sulfur diesel. To meet this low sulfur diesel level internally, refineries must have one or more of the following tools: distillate Hydrotreater, kerosene Hydrotreater, or Hydrocracker unit. In addition, if distil-

late from a fluid catalytic cracking unit FCC is to be used in diesel blending, either the FCC unit feed or distillate products should be hydrotreated.

Building a Hydrotreater unit is a significant investment that can cost anywhere from two hundred million to more than half a billion dollars, depending on the unit's capacity, location and processing flexibility. As diesel-powered public transportation is the main means of transportation in most developing countries, diesel prices can be seriously affected by such a move toward a lower diesel specification, requiring a huge investment. On the other hand, many large cities and capitals in developing countries are suffering from pollution generated by diesel-fueled vehicles such as buses and trucks. This makes it even more essential to implement a sulfur phase-out program, starting from the areas most affected. A similar case in the US is the Los Angeles basin area, where the pollution is severe but unique, thus necessitating California to implement more stringent environmental limits than those at the national level.

Results

The results demonstrated a reverse exponential decrease in the global objective with the reduction in sulfur level, as shown in Figure VIII-7. This is usually due to the higher cost of intermediate blending stocks required to produce the lower sulfur diesel, in addition to the higher operating cost of process units such as Hydrotreaters. The effects of environmental objectives represented as upgrades in product specs in this case is clearly nonlinear and closer to an exponential effect.

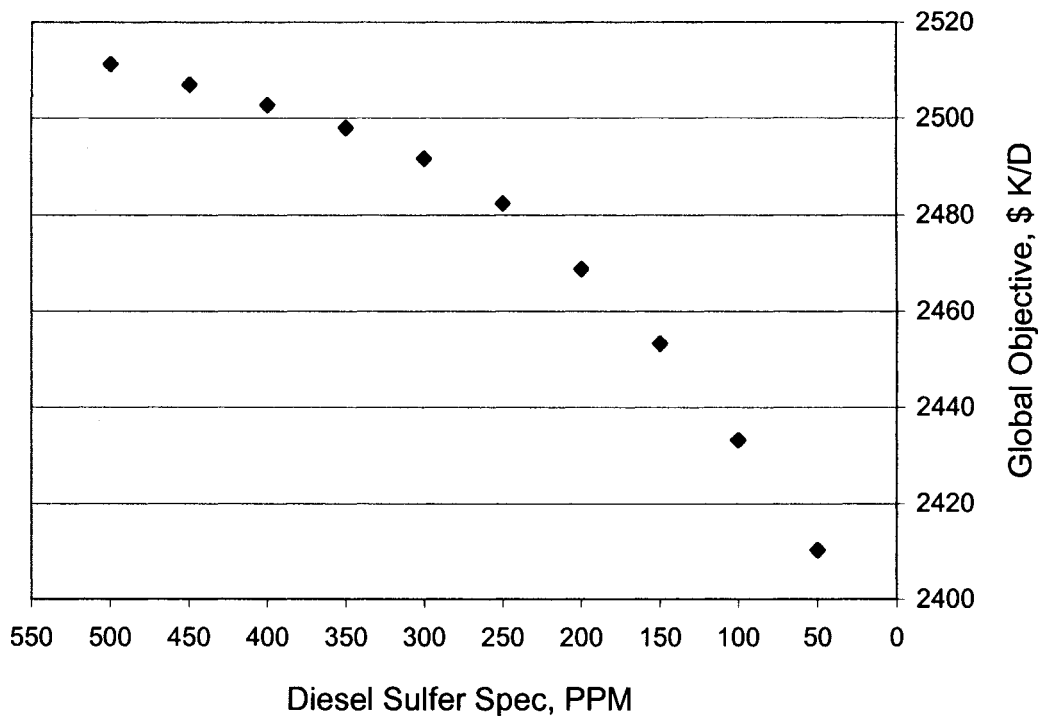


Figure VIII-7: Environmental Objective Effect—Global Diesel Sulfur Phase-Out: Nonlinear Effect on Global Objective

When considering the Environmental Objective Effect on specific refineries, it was noted that each refinery experienced different effects depending on its process limitations. For example, for Refinery # 4, the extra hydrotreating capacity requirements increased linearly up to the 150 PPM level. After that, the extra hydrotreating requirements increased considerably but in a linear manner with a high sloping line, as can be seen in Figure VIII-8. This suggests an optimum desulphurization level for that particular refinery of 150 PPM sulfur. This may be taken into consideration when deciding to upgrade the product spec. This refinery can be upgraded only to produce 150 PPM sulfur diesel. If the national spec

is higher than this in sulfur, the product of this refinery can be sent as a blending component to other refineries lacking hydrotreating capacity. If the national sulfur spec requires a lower sulfur level, then the refinery may operate at 150 PPM sulfur and study the benefit of importing some lower sulfur diesel as a blending component.

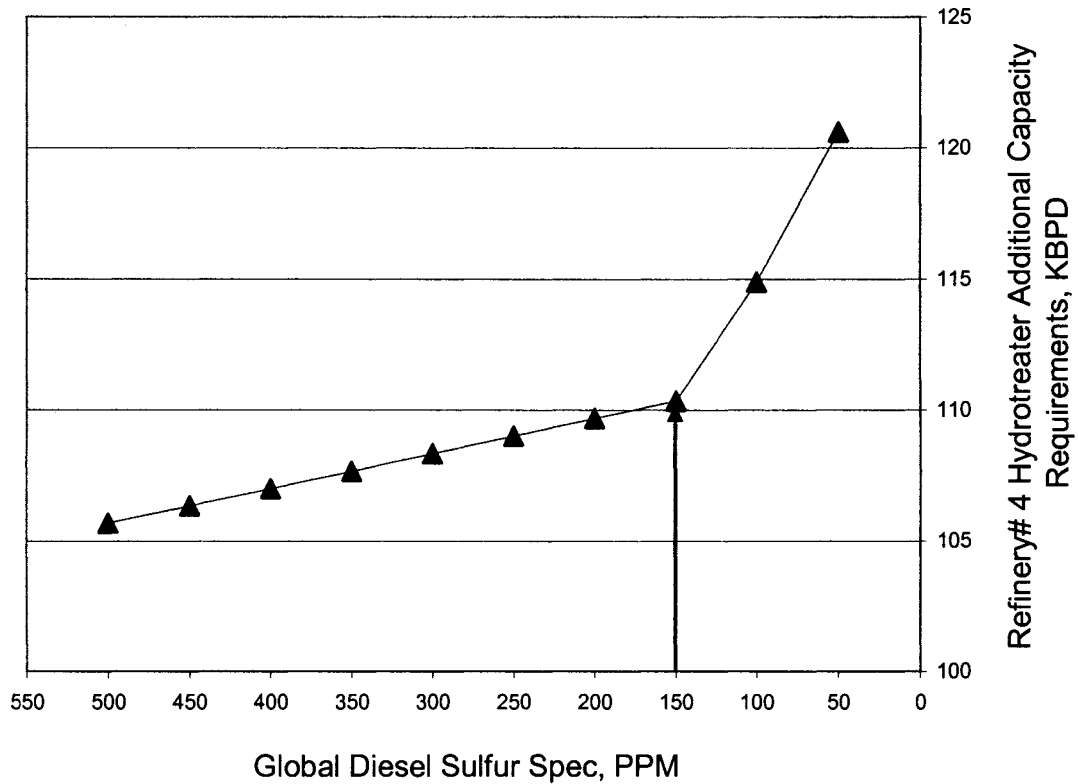


Figure VIII-8: Environmental Objective Effect—Global Diesel Sulfur Phase-Out: Optimum Desulphurization Level at 150 PPM

The results demonstrated a need for additional hydrotreating capacities at some refineries. This may constitute a problem, since it is to be attained by one of the following methods:

1. Raising the unit charge rate if extra capacity exists. However, this will reduce the cycle length and increase operating costs.
2. Commissioning of an idle unit, as was the case for the refinery that had a large distillate Hydrotreater and a small kerosene Hydrotreater. Economics usually suggests operating one unit with the lower operating cost instead of operating two units simultaneously. In this case, the larger unit was the distillate Hydrotreater. However, with more demand for low sulfur blending stokes, the other unit had to be re-commissioned. Another factor of importance is the product quality of each unit—that is, the sulfur content and throughput each unit can produce. There is a maximum limit for the amount of kerosene that can be blended with diesel, which is in turn limited by the final diesel flashpoint and, in rare cases, by the distillation.
3. Simple revamping of the existing unit. This may cost anywhere from several million to tens of millions of dollars. The economics depends on the scope of the revamp. For example, the unit may be bottlenecked by the amount of cooling of a certain product, which may be solved by installing a new heat exchanger or utilizing an idle one. Usually the maximum additional capacity attainable from any revamp is about 30% of the maximum unit throughput. Due to the nature of the hydrotreating units and high pressures of about 2000 pounds per square inch (PSI), the equipment cost is substantial and requires special materials and welding procedures.
4. A grass roots unit which, as mentioned above, can cost hundreds of millions of dollars. Usually this is the last alternative a refinery would con-

sider. If a refinery management has the means, it would rather utilize available funds to build a profitable unit such as a CCR or an FCC that can produce a significant profit gain in the refinery margin.

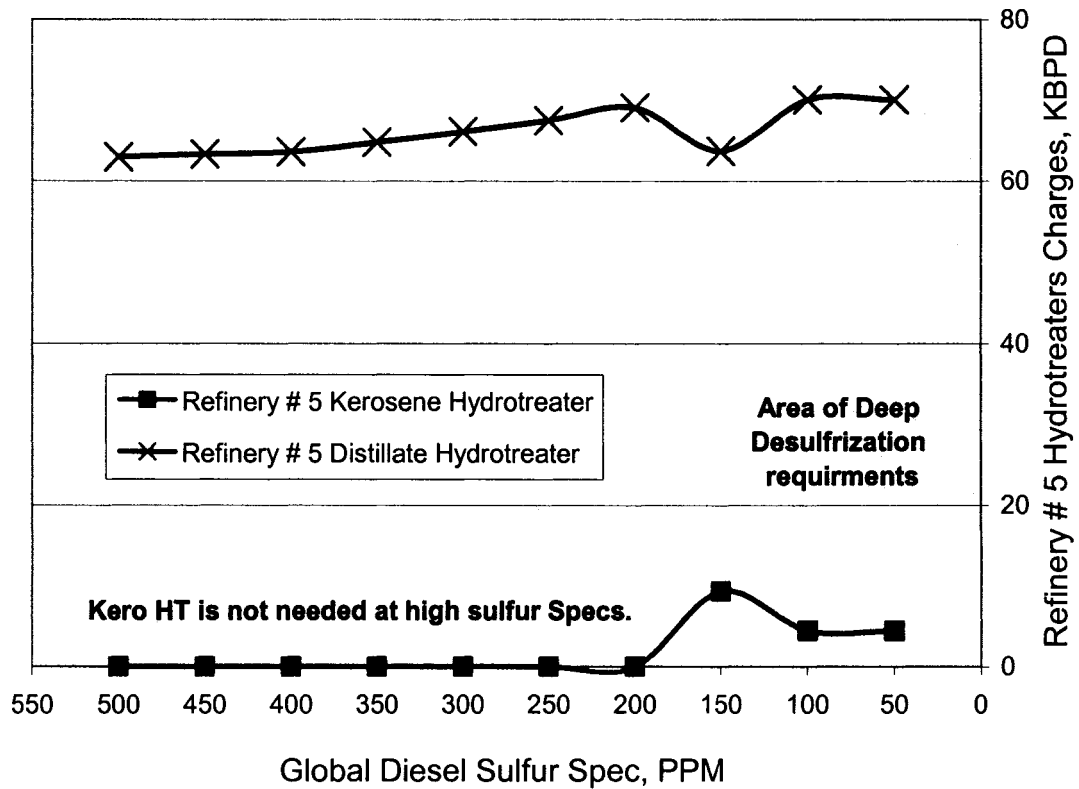


Figure VIII-9: Environmental Objective Effect--Global Diesel Sulfur Phase-Out: Hydrotreating Capacity Requirements to meet the 50 PPM Sulfur Diesel Spec

Refinery # 2, which is an inland facility, had to dump unblendable diesel into asphalt due to the limitations of the market for fuel oil. However, asphalt spec is more sensitive than fuel oil to viscosity and only a limited amount of diesel can be dumped into asphalt. After that, the asphalt may become so soft that it loses its curing and hardness specifications.

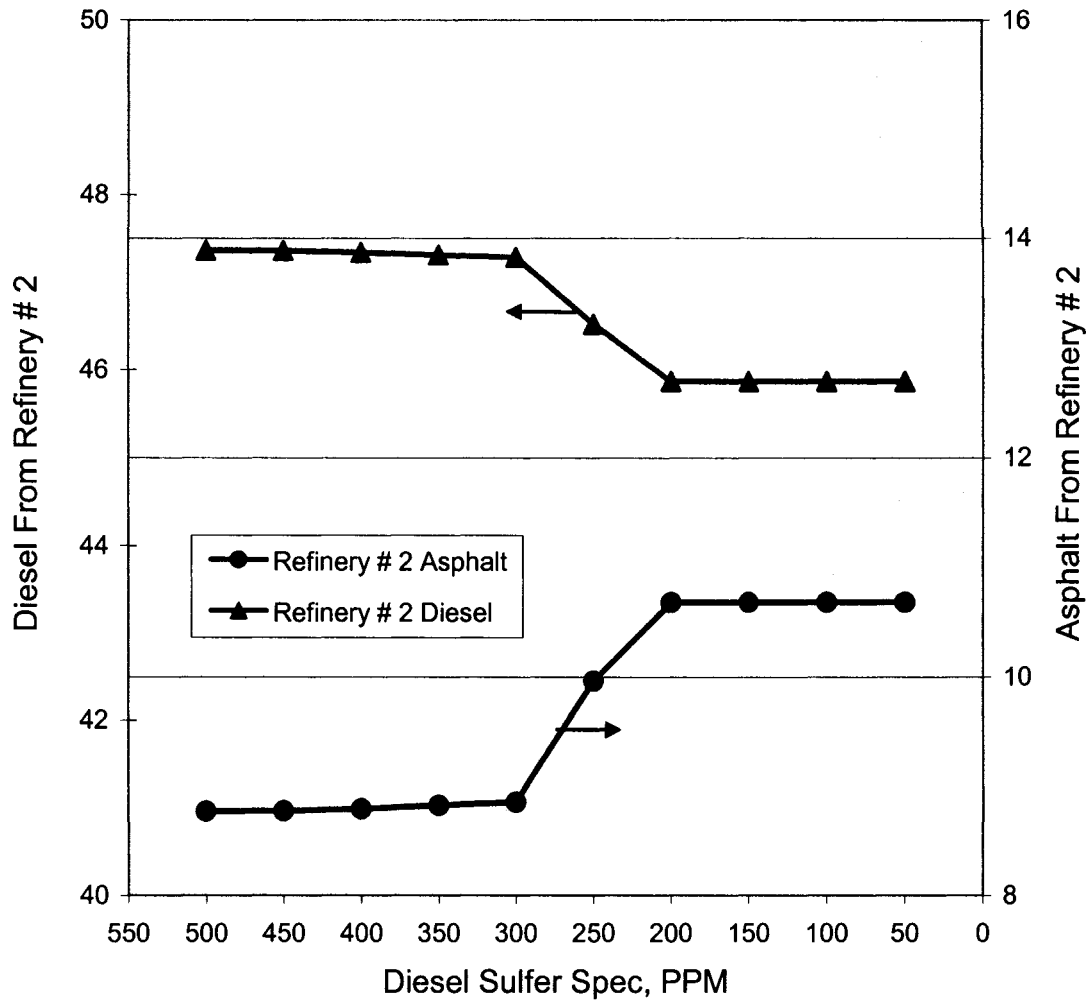


Figure VIII-10: Environmental Objective Effect—Global Diesel Sulfur Phase-Out: High Sulfur-Diesel Blending Components Dumped into Asphalt in an In-Land Refinery

It worth mentioning that when comparing objectives, we are comparing the trend in each objective not the absolute values, since the objective function of each refinery is set differently and can be custom-made for the global objective

function. This is similar to dealing with enthalpies in which the important aspect is the enthalpy difference or enthalpy relative to a reference point.

VIII.2. ENVIRONMENTAL AND PRODUCT SPEC OBJECTIVES

CONCLUSION

1. Most of the observations concerning objective cases of catastrophic failure effects apply to environmental objective cases, as discussed below.
2. As observed in catastrophic failure objective cases, the results indicated that refineries can have a local multi objective optimum that does not necessarily favor the global objective or even the local single objective optimum.
3. The relationship between the global and local optimum may not always be linear. Moreover, the two objectives may not necessarily move in the same direction or at the same rate. This is the same phenomenon that was observed in the catastrophic failure effects objective runs.
4. For refineries, the multi objective local optimum may be different from the local optimum for the purely economic objective case as discussed in the catastrophic failure effects section.
5. Refineries exhibited smoother behavior in capacity or local objective changes as a result of imposed constraints as compared to more discrete behavior in the case of the catastrophic failure objective. The global objective exhibited smooth behavior in both cases.

6. The environmental objective effect on refinery operations and the local objective was less significant than the catastrophic failure effect objective. One reason is that refineries can still produce under environmental objective constraints even though some products may be degraded—for example, dumping diesel to fuel oil. In the case of catastrophic failure, the operations are closer to an on/off operation by which the refinery may lose a minimum of 25 % of its capacity in one step, assuming that only one train is affected, which makes the effect on objectives and production capacity more significant for refinery operations.
7. Different refineries had different levels beyond which the effect of the environmental objective increased sharply. For example, one refinery demonstrated an optimum level at 150 PPM sulfur diesel spec, while another showed a huge drop in the objective and capacity after 300 PPM. This should be taken into consideration when deciding to upgrade refineries.
8. The results demonstrated that the increase in Hydrotreating requirements is not linearly related to the decrease in product sulfur level. In some cases, the relationship was exponential, while in others it was close to exponential but having two different linear regions. This should be taken into consideration when revising product specs.
9. Refinery # 3 exhibited the same inverse relationship to the global objective as was the case for the catastrophic failure effects objective. This is due to the unique price structure and supply constraints imposed on this refinery.

IX OVERALL CONCLUSION

1. Most of the observations for catastrophic failure effects' objective cases apply to environmental objective cases as well.
2. The results for all cases showed that refineries can have a local multi objective optimum that is not necessarily in favor of the global objective or even of the local single objective optimum as discussed below. It was also shown that the relationship between global and local optimums may not always be linear. Moreover, the two objectives may not necessarily move in the same direction or at the same rate. This is a factor related to the internal complexities of refineries and the types of imposed constraints.
3. For refineries, the multi objective local optimum may differ from the local optimum in purely economic objective cases. The amount of deviation from the pure economic optimum depends on the degree of flexibility of the refinery, both in selecting different feed/product schemes and in having different operating modes. These flexibilities act as a relief on the imposed multi objective constraints by providing more alternatives to the model, which increases the feasible region and thus may lead to a more optimal solution.

4. For the catastrophic failure effects, the change in the capacity or the local objective as a result of imposed constraints usually follows a discrete behavior pattern in contrast to the environmental objective cases where the effect is smoother. The global objective normally follows a smooth curve.
5. For the catastrophic failure effects objective, crude processing capacity is the main factor. The loss of feed-processing capacity such as crude or condensate had a greater effect on the objectives than the loss of upgrading and treatment capacities such as gasoline reforming.
6. The catastrophic failure effects objective results demonstrated the benefit of having more than one crude unit, which gives greater flexibility in running the refinery in less than the 60 % minimum turndown ratio.
7. The catastrophic failure effects objective results demonstrated the importance of examining the effects of loss of internal processing flexibility on product supplies, which may not be clear in either local or global objective functions but will appear at the point at which supply needs cannot be met from all the local refineries and thus imports are needed.
8. For all objectives, the price structure of Refinery # 3 creates a conflict with the global objective on some points. This is due to constraints imposed on the refinery to meet the demand for both the nearby lube refinery and the local urban market without crediting the refinery's local objective for sacrificing its own optimum to meet these demands.
9. The environmental objective effect on refinery operations and local objectives was less significant than the catastrophic failure effect objective.

This is due to the fact that refineries can still produce under environmental objectives even though some products may be degraded, whereas in the catastrophic failure effects objective, the refinery may lose a minimum of 25% of its capacity in one step, which has more effect on objectives and production capacity.

10. Environmental objective results demonstrated that the increase in hydrotreating requirements is not linearly related to the decrease in product sulfur level.

X RECOMMENDATIONS

1. It is recommended that this work be extended using optimization techniques other than traditional LP and NLP for areas that showed a nonlinear relationship between the global and local objectives. These techniques include genetics algorithms.
2. It is recommended to examine the possibility of modeling the refineries and markets as nodes in a neural network model and then enter the results of this work. The neural net should then be trained for different scenarios. A completely trained network should then be studied for applicability in predicting future events and recommending solutions.
3. The price structure of refineries and markets should be re-evaluated to reflect the strengths and constraints of each refinery. Refineries that are required to meet certain demands that are not in the refinery's interest should be recompensed. For example, if a refinery is required to produce very low sulfur diesel in order to meet certain market demands, although this costs more to the refinery, which has the ability to manufacture other profitable products, credit should be extended to the refinery's objective to compensate it for its loss of revenue. This could be calculated as the difference between the refinery's actual revenue and the revenue it would earn if it operated under its own optimum operating scheme.

4. In searching for and making a decision concerning an optimization, care should be taken not to depend solely on monitoring objectives. The results of this work demonstrate that product shortages may not appear in either objective until imports become a necessity. Appropriate import tiers should be implemented to deal with this effect.
5. When deciding to upgrade the products spec (or even to upgrade refineries), the effect of the new product spec on each refinery should be examined to determine the processing optimum for that refinery. For example, the optimum for some refineries was at 150 PPM sulfur, while for others the optimum was at 300 PPM. It may be optimum at the global level to set the spec at a point between these two limits and have products from both refineries blended together to form a final blend that just meets the spec. It may be possible to construct a large treating unit at a refinery which costs less than constructing smaller units at different refineries. Sensitivity analysis and long term transportation pricing should be considered in the decision.

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