Petroleum Refining and Petrochemical Industry Integration and Coordination under Uncertainty

by

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Khalid Yahya Al-Qahtani

Abstract

Petroleum refining and the petrochemical industry account for a major share in the world energy and industrial market. In many situations, they represent the economy back-bone of industrial countries. Today, the volatile environment of the market and the continuous change in customer requirements lead to constant pressure to seek opportunities that properly align and coordinate the different components of the industry. In particular, petroleum refining and petrochemical industry coordination and integration is gaining a great deal of interest. However, previous research in the field either studied the two systems in isolation or assumed limited interactions between them.

The aim of this thesis is to provide a framework for the planning, integration and coordination of multisite refinery and petrochemical networks using proper deterministic, stochastic and robust optimization techniques. The contributions of this dissertation fall into three categories; namely, a) Multisite refinery planning, b) Petrochemical industry planning, and c) Integration and coordination of multisite refinery and petrochemical networks.

The first part of this thesis tackles the integration and coordination of a multisite refinery network. We first address the design and analysis of multisite integration and coordination strategies within a network of petroleum refineries through a mixed-integer linear programming (MILP) technique. The integrated network design specifically addresses intermediate material transfer between processing units at each site. The proposed model is then extended to account for model uncertainty by means of two-stage stochastic programming. Parameter uncertainty was considered and included coefficients of the objective function and right-hand-side parameters in the inequality constraints. Robustness is analyzed based on both model robustness and solution robustness, where each measure is assigned a scaling factor to analyze the sensitivity of the refinery plan and the integration network due to variations. The proposed technique makes use of the sample average approximation (SAA) method with statistical bounding techniques to give an insight on the sample size required to give adequate approximation of the problem.

The second part of the thesis addresses the strategic planning, design and optimization of a network of petrochemical processes. We first set up and give an overview of the

deterministic version of the petrochemical industry planning model adopted in this thesis. Then we extend the model to address the strategic planning, design and optimization of a network of petrochemical processes under uncertainty and robust considerations. Similar to the previous part, robustness is analyzed based on both model robustness and solution robustness. Parameter uncertainty considered in this part includes process yield, raw material and product prices, and lower product market demand. The Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) are also investigated to numerically illustrate the value of including the randomness of the different model parameters.

The final part of this dissertation addresses the integration between the multisite refinery system and the petrochemical industry. We first develop a framework for the design and analysis of possible integration and coordination strategies of multisite refinery and petrochemical networks to satisfy given petroleum and chemical product demand. The main feature of the work is the development of a methodology for the simultaneous analysis of process network integration within a multisite refinery and petrochemical system. Then we extend the petroleum refinery and petrochemical industry integration problem to consider different sources of uncertainties in model parameters. Parameter uncertainty considered includes imported crude oil price, refinery product price, petrochemical product price, refinery market demand, and petrochemical lower level product demand. We apply the sample average approximation (SAA) method within an iterative scheme to generate the required scenarios and provide solution quality by measuring the optimality gap of the final solution.

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Nomenclature

Indices

cfr	refinery final product
cir	refinery intermediate stream
cp	petrochemical commodity
cr	refinery raw material
i	plant
j	iterations in the SAA method
k	scenario
m	production unit
p	refinery process operating mode
q	quality specification
rf	refinery fuel
s	refinery units predetermined expansion size

Sets

CB	streams for blending refinery products
CFP	petrochemical final products
CFR	refinery final products
CIP	petrochemical intermediate streams
CIR	refinery intermediate streams
CP	petrochemical commodities
CR	refinery raw materials
FUEL	streams comprising refinery fuel
I	plants

M_{Pet}	petrochemical units
M_{Ref}	refinery units
N	number of samples donating the sample size in the optimality gap bounding calculation using SAA method
NRF	non-refinery petrochemical feed
P	refinery process operating modes
PEX	products for exports
Qv	quality of products that blends by volume
Qw	quality of products that blends by weight
R	number of sample batches donating the number of replications in the optimality gap bounding calculation using SAA method
RF	refinery fuel streams
RPF	refinery finals products as petrochemical feed
RPI	refinery intermediates as petrochemical feed
S	refinery unties predetermined expansion sizes

Parameters

$\alpha_{cr,cir,i,p}$	refinery input-output coefficients of intermediate stream *cir* from crude *cr* at plant *i* by process *p*
$\beta_{cr,rf,i,p}$	refinery fuel consumption coefficients of refinery fuel *rf* from crude *cr* at plant *i* by process *p*
$\gamma_{m,p}$	refinery assignment of process operating mode *p* to equipment *m*
$\delta_{cp,m}$	petrochemical input-output coefficients of commodity *cp* in process *m*
$\xi_{cr,cir,i,p,i'}$	refinery integration superstructure of all possible alternatives to transfer crude *cr* of commodity *cir* from plant *i* to process *p* in plant *i'*
$AddC_{m,i}$	additional capacity of production unit *m* at plant *i*

$att_{cr,cir,q}$	attributes of intermediate streams *cir* produced from crude *cr* blending of property q
B_m^L	petrochemical process minimum economic capacity
C_{cp}^{Pet+}	shortfall penalty cost of each unit of a product $cp \in CFP$
C_{cp}^{Pet-}	surplus penalty cost of each unit of a product $cp \in CFP$
C_{cfr}^{Ref+}	shortfall penalty cost of each unit of a product *cfr*
C_{cfr}^{Ref-}	surplus penalty cost of each unit of product *cfr*
$CrCost_{cr}$	deterministic price of crude *cr*
$CrCost_{cr,k}$	stochastic price of crude *cr* at scenario *k*
$cv_{rf,cir,i}$	refinery caloric value equivalent of refinery fuel *rf* by commodity *cir* at plant *i*
$D_{Pet}{}_{cp}^{L}$	petrochemical lower deterministic demand of product $cp \in CFP$
$D_{Pet}{}_{cp}^{U}$	petrochemical upper deterministic demand of product $cp \in CFP$
$D_{Pet}{}_{cp,k}^{L}$	petrochemical lower stochastic demand of product $cp \in CFP$ at scenario k
$D_{Ref}{}_{cfr}$	refinery deterministic demand of products *cfr*
$D_{Ref}{}_{cfr,k}$	refinery stochastic demand of product *cfr* at scenario *k*
$F_{cir,i,i'}^{U}$	flowrate upper bound of intermediate *cir* from plant *i* to *i'*
IM_{cr}^{U}	import upper bound level of commodity *cr*
IM_{cr}^{L}	import lower bound level of commodity *cr*
$InCost_{i,i'}$	insulation cost of piping to transfer refinery commodity *cir* from plant *i* to plant *i'*

$InCost_{m,s}$ installation cost of a refinery production unit *m*

K^U petrochemical process production upper bound

$MaxC_{m,i}$ maximum capacity of production unit *m* at plant *i*

$MinC_{m,i}$ minimum capacity required of production unit *m* at plant *i*

$OpCost_p$ refinery operating cost of process *p*

p_k probability of scenario *k*

Pr_{cp}^{Pet} deterministic price of petrochemical commodity *cp*

$Pr_{cp,k}^{Pet}$ stochastic price of petrochemical commodity *cp*

Pr_{cfr}^{Ref} deterministic export price of product c*fr*

$Pr_{cfr,k}^{Ref}$ stochastic price of product *cfr* at scenario *k*

$q_{cir,q}^{L}$ quality bounds of commodity *cir* of property q

$q_{cir,q}^{U}$ upper level bounds of commodity *cir* of property q

S_{cp}^{Pet} non-refinery petrochemical feed supply of commodity $cp \in NRF$

$sg_{cr,cir}$ specific gravity of commodity *cir* by crude *cr*

Variables

$\widetilde{\varepsilon}_u$ error estimate of upper bound objective function

$\widetilde{\varepsilon}_l$ error estimate of lower bound objective function

$\frac{\sigma^2_{\bar{v}_N}}{R}$ variance estimator of the upper bound objective function

$\frac{\sigma^2_{\hat{v}_{N'}}}{N'}$ variance estimator of lower bound objective function

v_N^j	objective function value of each iteration j with a sample size N
$\overline{v}_N$	objective function upper bound estimator over a sample size N
$\hat{v}_{N'}$	objective function lower bound estimator (point estimator) over a sample size N
$e_{cfr',i}^{Ref}$	refinery exports of final product $cfr \in PEX$ from refinery i
$Ff_{cr,cp,i}^{Pet}$	petrochemical feed from refinery final product $cfr \in RPF \in CP$ from plant i
$Fi_{cr,cp,i}^{Pet}$	petrochemical feed from refinery intermediates $cir \in RPI \in CP$ form plant i
Fn_{cp}^{Pet}	petrochemical feed from non-refinery commodity cp
$S_{cr,i}^{Ref}$	refinery supply of raw material cr to refinery i
$V_{cfr,k}^{Ref+}$	shortfall of product cfr at scenario k
$V_{cfr,k}^{Ref-}$	surplus of product cfr at scenario k
$V_{cp,k}^{Pet+}$	shortfall of product $cp \in CFP$ at scenario k
$V_{cp,k}^{Pet-}$	surplus of product $cp \in CFP$ at scenario k
$w_{cr,cir,cfr,i}$	blending levels of crude cr that produces intermediate cir to yield a product cfr at plant i
x_m^{Pet}	mass flowrate of petrochemical production unit m
$x_{cfr,i}^{Ref}$	mass flowrate of refinery final product cfr by refinery i
xi_{cp}^{Pet}	mass flow rate of petrochemical intermediate stream $cp \in CIP$
$xi_{cr,cir,i,p,i'}^{Ref}$	refinery transshipment level of crude cr of commodity cir from plant i to process p at plant i'
$xv_{cfr,i}^{Ref}$	volumetric flowrate of refinery final product cfr by refinery i
$y_{exp}{}_{m,i,s}^{Ref}$	binary variable representing refinery expansions of production unit m at plant i for a specific expansion size s

$y_{pipe}^{Ref}_{cir,i,i'}$ binary variable representing transshipment of refinery commodity *cir* from plant *i* to plant *i'*

$y_{proc}^{Pet}_{m}$ binary variable representing petrochemical selection of unit *m*

$z_{cr,p,i}$ process input flowrate of crude *cr* to process *p* at plant *i*

Processing Unit

DATK	Desulfurization of aviation turbine kerosene
DCG	Desulfurization of cycle gas oil
DCK	Delayed coker
DGO	Desulfurization of gas oil
CDU	Crude distillation
DIST	Desulfurization of delayed coker distillates
FCC1	Fluid catalytic cracker (gasoline mode)
FCC2	Fluid catalytic cracker (gas oil mode)
HCU	Hydrocracker
ISOM	Isomerization
REF1	Reformer (95% severity)
REF2	Reformer (100% severity)

Stream

100	Reformate at 100% severity
95	Reformate at 95% severity
ATK	Aviation turbine kerosene intermediates
ATKP	Aviation turbine kerosene product
C-4	C-4 fractions (mixed butanes, -enes, etc.)
CGO	Cycle gas oil

Cl	Chlorine
CN	Fluid catalytic cracker gasoline
CoGO	Coker gas oil
Coke	Petroleum coke
CR	Crude oil
DCGO	Desulfurized cycle gas oil
Diesl	Petroleum diesel product
DIST	Distillate
DSATK	Desulfurized aviation turbine kerosene
DSDIST	Desulfurized distillate
DSGO	Desulfurized gas oil
E	Ethylene
EDC	Ethylene dichloride
GO	Gas oil
GO6	No.6 gas oil
GSLN	Petrochemical gasoline
HCI	Hydrochloric acid
HFO	Petroleum heating fuel oil
HN	Heavy naphtha
ISO	Isomerate
JP4	No.4 jet fuel
KE	Kerosene
LN	Light naphtha
LPG	Liquefied petroleum gas
NaOH	Sodium hydroxide

P	Propylene
PFG	Petrochemical fuel gas
PFO	Petrochemical fuel oil
PG95	Refinery gasoline with 95 octane number
PG98	Refinery gasoline with 98 octane number
PVA	polyvinyl alcohol
PVC	Polyvinyl chloride
RF	Refinery fuel
RG	Refinery gas
T	Toluene
UCO	Unconverted gas oil
VCM	Vinyl chloride monomer
VGO	Vacuum gas oil
VRSD	Desulfurized vacuum residue

Acronyms

ATKP	Military Jet Fuel
BMCI	Bureau of Mines Correlation Index
BTX	Benzene-Toluene-Xylene
CVaR	Conditional Value-at-Risk
Des	Desulfurization
EEV	Expectation of Expected Value
EV	Expected Value
EVPI	Expected Value of Perfect Information
FCC	Fluid Catalytic Cracker
GAMS	General Algebraic Modeling System
GTI	Gas Turbine Integration
LP	Linear Programming
LSR	light Straight-Run
MAP	Method of Approximation Programming
MILP	Mixed-Integer Linear Programming
MINLP	Mixed-Integer Non-Linear Programming
MV	Mean-Variance
NLP	Non-Linear Programming
OTOE	One Task-One Equipment
Paygas	Pyrolysis Gasoline
PIMS	Process Industry Modeling System
RPMS	Refinery and Petrochemical Modeling System
SAA	Sample Average Approximation

SEN	State-Equipment Network
SLP	Successive Linear Programming
SRI	Stanford Research Institute
SS	Stochastic Solution
STN	State-Task Network
UPM	Upper Partial Mean
VaR	Value-at-Risk
VSS	Value of Stochastic Solution
VTE	Variable-Task Equipment
WS	Wait-and-See

Chapter 1

Introduction

1.1 Motivation

Petroleum refining and the petrochemical industry play a paramount role in the current world economy. They provide the platform to transform raw materials into many essential products in our life, ranging from transportation and industrial fuels to basic components for plastics, synthetic rubbers and many other useful chemical products. The economic growth and increasing populations will keep global demand for such products high for the foreseeable future. According to the International Energy Agency (IEA, 2006), petroleum makes up 42.3% of the total energy consumption in the world. One half of the petroleum consumption over the period of 2003 to 2030 will be in the transportation sector. The industrial sector, on the other hand, accounts for a 39% of the projected increase in world oil consumption, mostly in chemical and petrochemical processes (EIA, 2006). Meeting such demand will require large investments and proper optimization tools for the strategic planning of these industries.

The competition in the market place is another pressing motive for firms to pursue strategies in order to gain a competitive edge, including the search for opportunities to improve their coordination and synergy. Bhatnagar et al. (1993) defined two levels of coordination, namely: “general coordination” and “multiplant coordination”. The first class considers the problem of integrating different activities of the supply, production and

distribution. The second class, 'multiplant coordination", mainly addresses production planning problems. They stressed the importance and need to further develop and design general and clear frameworks for multiplant coordination. The benefits projected from the coordination of multiple sites are not only in terms of expenses but also in terms of market effectiveness and responsiveness (Shah, 1998). Most of the previous strategic planning studies have focused mainly on restricted defined supply chain networks and have not provided a thorough analysis of an enterprise as a whole (Shapiro, 2004). Furthermore, they focused on the coordination of the multiple system echelons of a firm where less attention was given to providing a framework for the coordination of the same planning level at multiple sites via process network integration.

However, considering such high level planning decisions, especially with the current volatile market environment, requires knowledge of uncertainties impact. In production planning, sources of system uncertainties can be categorized as short-term or long-term depending on the extent of time horizon (Subrahmanyam et al., 1994). The short-term uncertainties mainly refer to operational variations, equipment failure, etc. Whereas, long-term uncertainty may include supply and demand rate variability and price fluctuations, on a longer time horizon (Shah, 1998). Technological uncertainty in the left-hand-side coefficients which can be viewed in the context of production planning as the variation in process yields is another important uncertainty factor. Reklaitis (1991), Rippin (1993), Shah (1998), and Grossmann (2005) reviewed the development of the general planning and scheduling problems and summarized the main future challenges as 1) Development of effective integration and coordination of different planning and scheduling models on single and multisite systems, 2) Modeling uncertainty through adequate stochastic models, and 3)

Development of efficient and general purpose algorithms tailored to provide proper solution techniques for planning and scheduling problems.

All the above mentioned challenges stimulated the main thrust of this thesis with an ultimate objective of addressing the planning, integration and coordination of multisite refinery and petrochemical systems.

1.2 Contributions

The aim of this dissertation is to provide a framework for the planning, integration and coordination of multisite refinery and petrochemical networks using proper deterministic, stochastic and robust techniques. The contributions of this thesis are organized into three parts, addressing different components of the system and advance to achieve the overall thesis objective.

Multisite Refinery Planning

Currently, the petroleum industry is facing pressures to reduce their product fuel prices, in spite of the soaring oil prices, while maintaining a high profit margin. With this market environment, oil companies strive to seek opportunities to increase their resources utilization and profit. This requires appropriate decision-making tools to utilize all available resources not only on a single facility scale, but in the more comprehensive outlook of an enterprise-wide scale. Most of the pervious studies focused on the coordination between the different functions of an enterprise without exploiting integration alternatives within the same planning level across multiple sites.

The aim of this part of the thesis (Chapter 3) is to address the design and analysis of multisite integration and coordination strategies within a network of petroleum refineries using different crude combination alternatives. In addition, account for production capacity expansion requirements as needed. The main feature of this work is the development of a methodology for simultaneous analysis of process network integration alternatives in a multisite refining system through a mixed-integer linear programming (MILP) with the overall objective of minimizing total annualized cost. The network design specifically addresses intermediate material transfer between processing units at each site. The performance of the proposed model is tested on several industrial-scale examples to illustrate the economic potential and trade-offs involved in the optimization of the network. Although the methodology is applied on a network of refineries, it can be readily extended to cover other networks of continuous chemical processes.

In the next phase (Chapter 4), we consider the problem of multisite integration and coordination within a network of petroleum refineries under uncertainty and using robust optimization techniques. The framework of the simultaneous analysis of process network integration, proposed in Chapter 3, is extended to account for uncertainty in model parameters. Robustness is analyzed based on both model robustness and solution robustness, where each measure is assigned a scaling factor to analyze the sensitivity of the refinery plan and the integration network due to variations. The stochastic model is formulated as a two-stage stochastic MILP problem whereas the robust optimization is formulated as an MINLP problem with nonlinearity arising from modeling the risk components. Parameters uncertainty considered include coefficients of the objective function in terms of crude and final products prices as well as the right-hand-side parameters in the inequality constraints in

terms of demand. The proposed method makes use of the sample average approximation (SAA) method with statistical bounding techniques. The proposed model is tested on two industrial-scale studies of a single refinery and a network of complex refineries. Modeling uncertainty in the process parameters provided a practical perspective of this type of problem in the chemical industry where benefits not only appear in terms of economic considerations, but also in terms of improved resource utilization.

Petrochemical Industry Planning

The Petrochemical industry is a network of highly integrated production processes where products of one plant may have an end use or may also represent raw materials for other processes. This multiplicity gives rise to a highly complex structure which requires proper planning tools and consideration of the different alternatives for future developments. Consideration of uncertainty in such decisions is of a great deal of importance and interest by both the private companies and governments. Previous studies in the field have mainly considered the problem under deterministic assumptions or considered only part of the uncertainty in the process parameters.

In this part, we first set up and give an overview of the deterministic version of the petrochemical planning model (Chapter 5). Then we extend it to address the strategic planning, design and optimization of a network of petrochemical processes under uncertainty and robust considerations (Chapter 6). Robustness is analyzed based on both model robustness and solution robustness, where each measure is assigned a scaling factor to analyze the sensitivity each component. The stochastic model is formulated as a two-stage stochastic MILP problem whereas the robust optimization is formulated as an MINLP

problem with nonlinearity arising from modeling the risk components. Parameter uncertainty considered in this part includes process yield, raw material and product prices, and lower product market demand. The study shows that the final petrochemical network bears more sensitivity to variations in product prices as apposed to variations in market demand and process yields for scaling values that maintain the final petrochemical structure obtained form the stochastic model. The concept of Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) are also investigated to numerically illustrate the value of including the randomness of the different model parameters.

Integration and Coordination of Multisite Refinery and Petrochemical Networks

The integration of petroleum refining and petrochemical industries is attracting a whole lot of interest among many companies and governments. Pervious research in the field assumed either no limitations on refinery feedstock to the petrochemical industry or fixed the refinery production levels assuming an optimal operation while optimizing the petrochemical system.

In this part of the thesis (Chapter 7), we address the design of optimal integration and coordination of multisite refinery and petrochemical networks to satisfy given petroleum and chemical products demand. The refinery and petrochemical systems were modeled as mixed-integer problem with the objective of minimizing the annualized cost over a given time horizon among the refineries and maximizing the added value of the petrochemical network. The main feature of the work is the development of a methodology for the simultaneous analysis of process network integration within a multisite refinery and petrochemical system. This approach provides a proper planning tool across the petroleum

refining and petrochemical industry systems and achieves an optimal production strategy by allowing trade offs between the refinery and the downstream petrochemical market. The proposed methodology not only devises the integration network in the refineries and synthesizes the petrochemical industry, but also provides refinery expansion requirements, production and blending levels.

In the final phase of this dissertation (Chapter 8), we extend the petroleum refinery and petrochemical industry integration problem to consider different sources of uncertainties in the problem. Uncertainties in the model included imported crude oil price, refinery product price, petrochemical product price, refinery market demand, and petrochemical lower level product demand. The problem is modeled as an MILP two-stochastic problem. Furthermore, we apply the sample average approximation (SAA) method within an iterative scheme to generate the required scenarios. The solution quality is then statistically evaluated by measuring the optimality gap of the final solution. This optimization approach for the petroleum refining and petrochemical industry provides an appropriate scheme for handling what is considered as a backbone of many countries' economies.

Chapter 2

Refining and Petrochemical Industry Background

2.1 Production Planning and Scheduling

Planning and scheduling can be defined as developing strategies for the allocation of equipment, utility or labor resources over time to execute specific tasks in order to produce single or several products (Grossmann et al., 2001). In most research dealing with planning and scheduling, there seems to be no clear cut between the two. Hartmann (1998) and Grossmann et al. (2001) pointed out some of the differences between a planning model and a scheduling model. In a general sense, process manufacturing planning models consider high level decisions such as investment on longer time horizons. Scheduling models, on the other hand, are concerned more with the feasibility of the operations to accomplish a given number and order of tasks.

Planning problems can mainly be distinguished as strategic, tactical or operational, based on the decisions involved and the time horizon considered (Grossmann et al., 2001). The strategic level planning considers a time span of more than one year and covers a whole width of an organization. At this level, approximate and/or aggregate models are adequate and mainly consider future investment decisions. Tactical level planning typically involves a midterm horizon of few months to a year where the decisions usually include production, inventory and distribution. Operational level covers shorter periods of time spanning from

one week to three months where the decisions involve actual production and allocation of resources. For a general process operations hierarchy, planning is the highest level of command. As shown in Figure 2.1, enterprise wide planning provides production targets for each individual site where each site transforms the plans into schedules and operational/control targets.

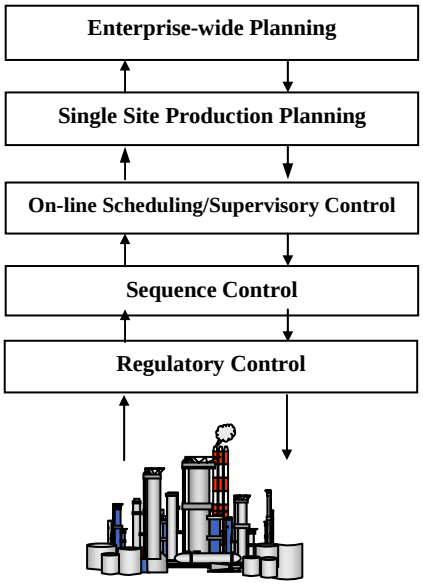

Figure 2.1 Process operations hierarchy. (Shah, 1998)

By any classification, proper communication between planning and scheduling activities on a single and an enterprise-wide system is still challenging. Review of the development of such hierarchal operations and their challenges are beyond the objective of this thesis. We refer interested readers to Reklaitis (1991), Rippin (1993), Shah (1998), and Grossmann (2005).

2.2 Petroleum Refining

2.2.1 Overview

The first refinery was built in Titusville, Pennsylvania in 1860 at a cost of $15,000 (Nelson, 1958). This refinery and other refineries at that time only used batch distillation to separate kerosene and heating oils from other crude fractions. During the early years, refining separation was performed using batch processing. However, with the increase in petroleum product demands, continuous refining became a necessity. The first widely recognized continuous refinery plants emerged around 1912 (Nelson, 1958). With the diversity and complexity of petroleum products demand, the refining industry has developed from a few simple processing units to very complex production systems. For a detailed history on the evolution of refining technologies, we refer the reader to Nelson (1958) and Wilson (1997).

A simplified process flow diagram of a typical modern refinery is shown in Figure 2.2. The refining processes can be divided into four main systems (OSHA, 2003):

- **Distillation Processes**. They are used to separate oil into fractions by distillation according to their boiling points. Distillation is usually divided into two steps, atmospheric and vacuum fractionation. This is done in order to achieve higher separation efficiencies at a lower cost.

- **Coking and Thermal Processes**. They convert heavy feedstocks, usually from distillation processes, to produce more desirable and valuable products that are suitable feeds to other refinery units. Such units include coking and visbreaking.

- **Catalytic Processes**. There are two types of catalytic conversion units in the refinery, cracking an alteration processes. Catalytic cracking converts heavy oils into lighter products that can be blended to produce high value final products, such as gasoline, jet fuels and diesel. Whereas, catalytic altering processes converts feedstocks to higher quality streams by rearranging their structures. These processes include reforming, alkylation and isomerization units. Catalytic processes produce hydrocarbon molecules with double bonds and form the basis of the petrochemical industry.

- **Treatment Processes**. They are applied to remove impurities, and other constituents that affect the properties of finished products or reduce the efficiency of the conversion processes. Typical examples of treating processes include desulfurizaiton, acid treating, and hydrotreating.

The atmospheric crude unit separates crude oil into several fractions including LPG, naphtha, kerosene, gas oil and residues. The heavy residues are then sent to the vacuum unit where they are further separated into vacuum gas oil and vacuum residues. Depending on the complexity and the refinery required production targets, different processing and treatment processes are applied to the crude fractions. Naphtha from the distillation unit is further separated into heavy and light naphtha. The heavy naphtha is sent to the catalytic reformer unit to produce high octane reformates for gasoline blending and the light naphtha is sent to light naphtha pool and to the isomerization unit to produce isomerate for gasoline blending as well. The middle distillates are combined with other similar intermediate streams and sent for hydrotreating and then blending to produce jet fuels and gas oils. Atmospheric and

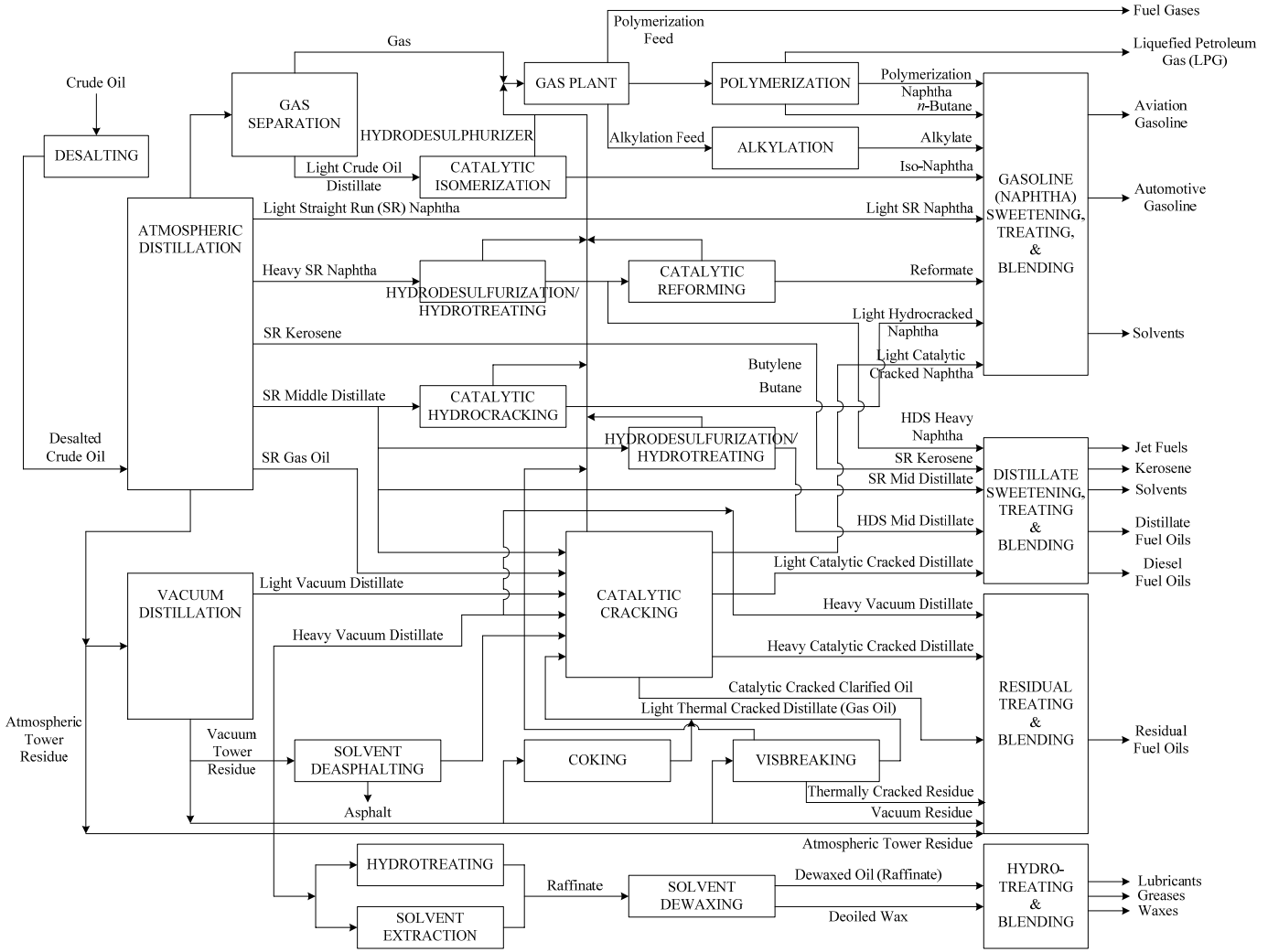

Figure 2.2 A simplified process flow diagram for a typical refinery. (Khor, 2007)

vacuum gas oils are further treated by catalytic cracking and in other cases by hydrocracking, or both, in order to increase the gasoline and distillate yields. In some refineries, vacuum residues are further treated using coking and thermal processes to increase light products yields. The above mentioned processes are highly complicated and involve different processing mechanisms. We refer the reader to standard petroleum refining textbooks, Gary and Handwerk (1994) for instance, for more details and process analysis.

2.2.2 Refinery Configuration

A refinery is made up of several distinct components that constitute a total production system, as shown in Figure 2.3. These components include:

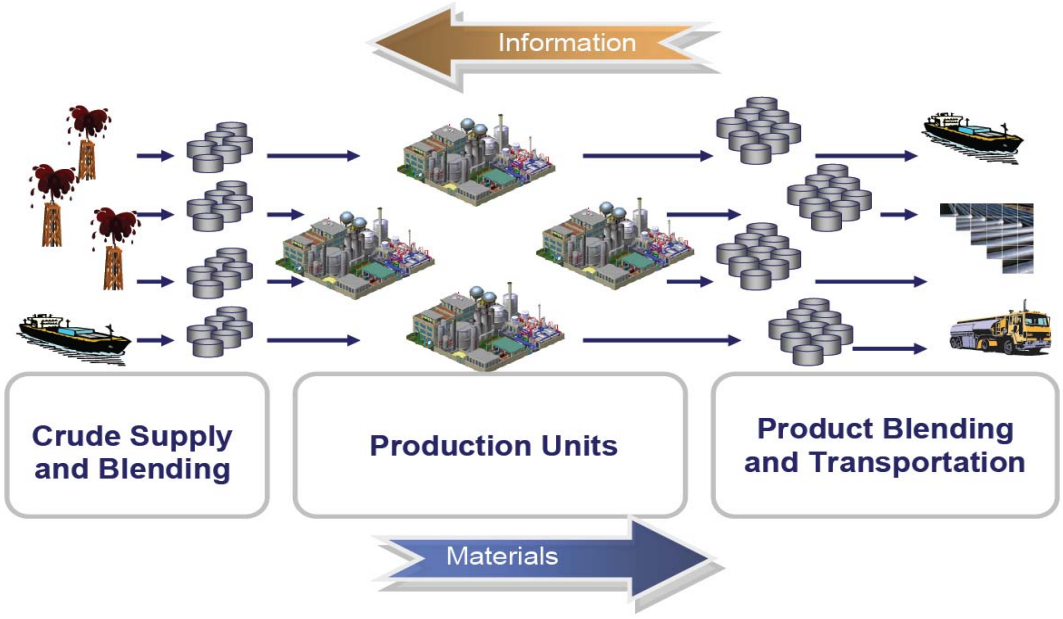

Figure 2.3 Schematic diagram of standard refining configuration.

- **Crude Supply and Blending.** This area includes receiving facilities and a tank area (tank farm) where all crude oil types are received and either blended or sent directly to the production system.

- **Production Units.** Production units separate crude oil into different fractions or cuts, upgrade and purify some of these cuts, and convert heavy fractions to light, more useful fractions. It also includes the utilities which provide the refinery with fuel, flaring capability, electricity, steam, cooling water, fire water, sweet water, compressed air, nitrogen, etc, all of which are necessary for the refinery's safe operation.

- **Product Blending and Transportation.** In this area final products are processed according to either a predetermined recipes and/or to a certain product specifications. This area also includes the dispatch (terminals) of finished products to the different customers.

The petroleum industry has long leveraged the use of mathematical programming and its different applications. The invention of both the simplex algorithm by Dantzig in 1947 and digital computers was the main driver for the wide spread use of linear programming (LP) applications in the industry (Bodington & Baker, 1990). Since then, many early applications followed in the area of refinery planning (Symonds, 1955; Manne, 1958; Charnes and Cooper, 1961; Wagner, 1969; Adams & Griffin, 1972) and distribution planning (Zierer et al., 1976).

One of the main challenges that inspired more research in the area of refining was the blending or pooling problem (Bodington & Baker, 1990). The inaccurate and inconsistent results from the use of linear blending relations led to the development of many techniques to handle nonlinearities. The nonlinearities arise mainly because product properties, such as octane number and vapor pressure assume a nonlinear relationship of quantities and properties of each blending component (Lasdon & Waren, 1983). In this context, we will

describe two commonly used approaches in industry and commercial planning softwares to tackle this problem. They are linear blending indices and successive linear programming (SLP).

Linear blending indices are dimensionless numerical figures that were developed to represent true physical properties of mixtures on either a volume or weight average basis (Bodington & Baker, 1990). They can be used directly in the LP model and span the most important properties in petroleum products, including octane number, pour point, freezing point, viscosity sulfur content, and vapor pressure. Many refineries and researchers use this approximation. Blending indices tables and graphs can often be found in petroleum refining books such as Gary and Handwerk (1994) or can be proprietarily developed by refining companies for their own use.

Successive linear programming (SLP), on the other hand, is a more sophisticated method to linearize blending nonlinearities in the pooling problem. The idea of SLP was first introduced by Griffith and Stewart (1961) of Shell Oil company where it was named the method of approximation programming (MAP). They utilized the idea of a Taylor series expansion to remove nonlinearities in the objective function and constraints then solving the resulting linear model repeatedly. Every LP solution is used as an initial solution point for the next model iteration until a satisfying criterion is reached. Bounding constraints were added to ensure the new model feasibility. Following their work, many improvement heuristics and solution algorithms were developed to accommodate bigger and more complex problems (Lasdon & Waren, 1980). Most commercial blending softwares and computational tools nowadays are based on SLP, such as RPMS by Honeywell Process Solutions (previously Booner & Moore, 1979) and PIMS by Aspen Technology (previously Bechtel

Corp., 1993). However, such commercial tools are not built to support studies on capacity expansion alternatives, design of plants integration and stochastic modeling and analysis.

All in all, the petroleum industry has invested considerable effort in developing sophisticated mathematical programming models to help planners provide overall planning schemes for refinery operations, crude oil evaluation, and other related tasks.

2.3 Petrochemical Industry

2.3.1 Overview

The Petrochemical industry is a network of highly integrated production processes. The products of one plant may have an end use but may also represent raw materials for another process. Most chemicals can be produced by many different sequences of reactions and production processes. This multiplicity of production schemes offers the sense of switching between production methods and raw materials utilization.

Petroleum feedstock, natural gas and tar represent the main production chain drivers for the petrochemical industry (Bell, 1990). From these, many important petrochemical intermediates are produced including ethylene, propylene, butylenes, butadiene, benzene, toluene, and xylene. These essential intermediates are then converted to many other intermediates and final petrochemical products constructing a complex petrochemical network. Figure 2.4 depicts a portion of the petrochemical alternative routs to produce cellulous acetate.

Figure 2.4 is in fact a small extraction of much larger and comprehensive flow diagrams found in Stanford Research Institute (SRI) reports. Note that certain chemicals,

Acetaldehyde and Acetic acid for example, appear in more than one place in the flowchart. This reflects the different alternatives of production routes available for most chemicals. In the industry, many chemicals are products of more than one process alternative, depending upon local conditions, corporate polices, and desired by-products (Bell, 1990).

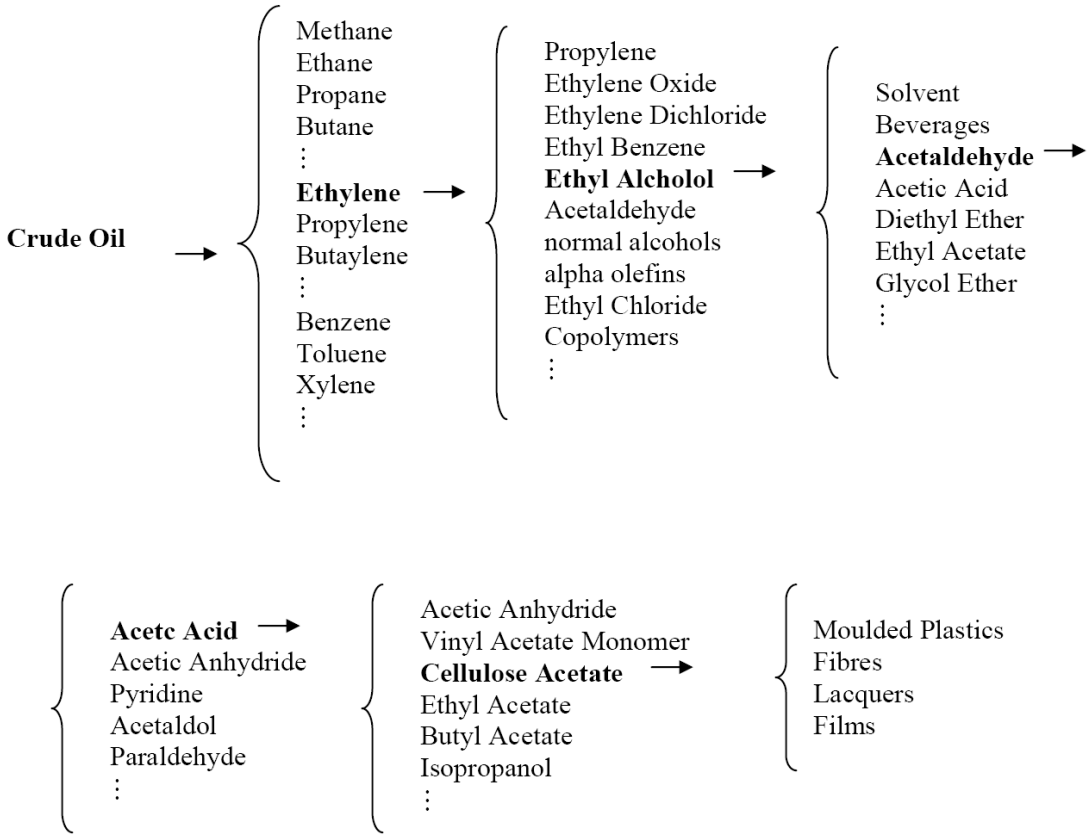

Figure 2.4 A Single Route of petroleum feedstock to petrochemical products. (Bell, 1990)

The flexibility in the petrochemical industry production and the availability of many process technologies require adequate strategic planning and a comprehensive analysis of all possible production alternatives. Therefore a model is needed to provide the development plan of the petrochemical industry. The model should account for market demand variability, raw material and product price fluctuations, process yields inconsistencies, and adequate incorporation of robustness measures.

The realization of the petrochemical planning need and importance has inspired a great deal of research in order to devise different models to account for the overall system optimization. Optimization models include continuous and mixed-integer programming under deterministic or parameter uncertainty considerations. Related literature is reviewed at a later stage of this thesis based on the chapter topic.

2.3.2 Petrochemical Feedstock

The preparation of intermediate petrochemical streams requires different processing alternatives depending on the feedstock quality. In our classification of petrochemical feedstocks we closely follow the one by Gary and Handwerk (1994) consisting of aromatics, olefins, and paraffins/cyclo-paraffins compounds. The classification of petrochemical feedstocks into these clusters helps identify the different sources in the refinery that provide suitable feedstock and therefore better recognize areas of synergy between the refinery and petrochemical systems.

2.3.2.1 Aromatics

Aromatics are hydrocarbons containing a benzene ring which is a stable and saturated compound. Aromatics used by the petrochemical industry are mainly benzene, toluene, xylene (BTX) as well as ethylbenzene and are produced by catalytic reforming where their yield would increase with the increase of reforming severity (Gary & Handwerk, 1994). Extractive distillation by different solvents, depending on the chosen technology, is used to recover such compounds. BTX recovery consists of an extraction using solvents that enhances the relative volatilities of the preferred compound followed by a separation process based on the products' boiling points. Further processing of xylenes using

isomerization/separation processes is commonly required to produce o-, m-, and p-xylene mixtures depending on market requirements. Benzene, in particular, is a source to a wide variety of chemical products. It is often converted to ethylbenzene, cumene, cyclohexane, and nitrobenzene which in turn are further processed to other chemicals including styrene, phenol, and aniline (Rudd et al., 1981). Toluene production, on the other hand, is mainly driven by benzene and mixed xylenes demand. Mixed xylene, particularly in Asia, is used for producing para-xylene and polyester (Balaraman, 2006).

The other source of aromatics is the pyrolysis gasoline (pygas) which is a byproduct of naphtha or gas oil steam cracking. This presents an excellent synergistic opportunity between refinery, BTX complex and stream cracking for olefins production.

2.3.2.2 Olefins

Olefins are hydrocarbon compounds with at least two carbon atoms having a double bond where their unstable nature and tendency to polymerize makes them one of the very important building blocks for the chemical and petrochemical industry (Gary & Handwerk, 1994). Although olefins are produced by fluid catalytic cracking in refineries, the main production source is through steam cracking of liquefied petroleum gas (LPG), naphtha or gas oils.

The selection of steam cracker feedstock is mainly driven by market demand as different feedstocks qualities produce different olefins yields. One of the commonly used feed quality assessment methods in practice is the Bureau of Mines Correlation Index (BMCI) (Gonzalo et al., 2004). This index is a function of average boiling point and specific gravity of a particular feedstock. The steam cracker feed quality improves with a decrease in the BMCI

value. For instance, vacuum gas oil (VGO) has a high value of BMCI and therefore is not an attractive steam cracker feed. The commonly used feedstocks in industry are naphtha and gas oil.

Steam cracking plays an instrumental role in the petrochemical industry in terms of providing the main petrochemical intermediates for the down stream industry. The steam cracker olefin production includes ethylene, propylene, butylene and benzene. These intermediates are further processed into a wide range of polymers (plastics), solvents, fibres, detergents, ammonia and other synthetic organic compounds for general use in the chemical industry (Rudd et al., 1981). In a situation where worldwide demand for these basic olefins is soaring, more studies are being conducted to maximize steam cracking efficiency (Ren et al., 2006). An alternative strategy would be to seek integration possibilities with the refinery as they both share feedstocks and products that can be utilized to maximize profit and processing efficiency.

2.3.2.3 Normal Paraffins and cyclo-paraffins

Paraffin hydrocarbon compounds contain only single bonded carbon atoms which give them higher stability characteristics. Normal paraffin compounds are abundantly present in petroleum fractions but are mostly recovered from light straight-run (LSR) naphtha and kerosene. However, the non-normal hydrocarbon components of LSR naphtha are of a higher octane number and therefore are preferred for gasoline blending (Meyers, 1997). For this reason, new technologies have been developed to further separate LSR naphtha into higher octane products that can be used in the gasoline pool and normal paraffins that is used as steam cracker feedstock (e.g. UOP IsoSiv^{TM} Process). The normal paraffins recovered

from kerosene, on the other hand, are mostly used in biodegradable detergents manufacturing.

Cyclo-paraffins, also referred to as naphthenes, are mainly produced by dehydrogenation of their equivalent aromatic compounds; such as the production of cyclo-hexane by dehydrogenation of benzene. Cyclo-hexane is mostly used for the production of adipic acid and nylon manufacturing (Rudd et al., 1981).

2.4 Refinery and Petrochemical Synergy Benefits

Process integration in the refining and petrochemical industry include many intuitively recognized benefits of processing higher quality feedstocks, improving value of byproducts, and achieving better efficiencies through sharing of resources. Table 2.1 illustrates different refinery streams that can be of superior quality when used in the petrochemical industry. The potential integration alternatives for refining and petrochemical industries can be classified into three main categories; 1) process integration, 2) utilities integration, and 3) fuel gas upgrade. The integration opportunities discussed below are for a general refinery and a petrochemical complex. Further details and analysis about the system requirements can be developed based on the actual system infrastructure, market demand, and product and energy prices.

2.4.1 Process Integration

The innovative design of different refinery processes while considering downstream petrochemical industry is an illustration of the realization of refining and petrochemical integration benefits. This is demonstrated by the wide varieties of refinery cracking and

reforming technologies that maximize olefin production. Some of the available technologies include cracking for high propylene and gasoline production (Fujiyama et al., 2005), maximum gasoline and LPG production, and low-pressure combination-bed catalytic reforming for aromatics (Wang, 2006). Other technologies include different extractive treatments of refinery streams, e.g. aromatic recovery from light straight-run (LSR) naphtha. The normal paraffins of the LSR, on the other hand, are typically used as a steam cracker feedstock (Meyers, 1997).

Table 2.1 Petrochemical alternative use of refinery streams. (Anon, 1998)

Refinery Stream	Petrochemical Stream	Alternative Refinery Use
FCC offgas	Ethylene	Fuel gas
Refinery propylene (FCC)	Propylene	Alkylation/polygasoline
Reformate	Benzene, toluene, xylenes	Gasoline blending
Naphtha and LPG	Ethylene	Gasoline Blending
Dilute ethylene (FCC & delayed coker offgas)	Ethylbenzene	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	o-xylene	Gasoline blending
Reformate	p-xylene	Gasoline blending
Kerosine	n-paraffins	Refinery product
FCC light cycle oil	Naphthalene	Diesel blending

Reforming, as mentioned above, is the main source of aromatics in petroleum refining where their yield increases with the increase in reforming severity. Aromatics in the reformate streams are recovered by extractive distillation using different solvents, depending on the chosen technology. The Benzene-Toluene-Xylenes (BTX) complex is one of the petrochemical processes that leverage a great deal of the integration benefits with petroleum

refining. The integration benefits are not only limited to the process side but extend to the utilities as will be explained in the following section.

Pyrolysis gasoline (pygas), a byproduct of stream cracking, can be further processed in the BTX complex to recover the aromatic compounds and the raffinate after extraction can be blended in the gasoline or naphtha pool (Balaraman, 2006). If there is no existing aromatics complex to further process the pygas, it could alternatively be routed to the reformer feed for further processing (Philpot, 2007). However this alternative may not be viable in general as most reformers run on maximum capacity. Pygas from steam cracking contains large amounts of diolefins which are undesirable due to their instability and tendency to polymerize yielding filter plugging compounds. For this reason, hydrogenation of pygas is usually recommended prior to further processing.

2.4.2 Utilities Integration (heat/hydrogen/steam/power)

Petroleum refining and the basic petrochemical industry are the most energy intensive processes in the chemical process industry (Ren et al., 2006). The energy sources in these processes assume different forms including fuel oil, fuel gas, electrical power, and both high and low pressure steam. The different energy requirements and waste from the whole range of refinery and petrochemical units present intriguing opportunities for an integrated complex. Integration of energy sources and sinks of steam cracking, for instance, with other industrial processes, particularly natural gas processing, can yield significant energy savings reaching up to 60% (Ren et al., 2006). Furthermore, gas turbine integration (GTI) between petrochemical units and ammonia plants can lead to a reduction in energy consumption by up to 10% through exhaust-heat recovery (Swaty, 2002). This can be readily extended to the

refinery processing units which span a wide variety of distillation, cracking, reforming, and isomerization processes.

Hydrogen is another crucial utility that is receiving more attention recently mainly due to the stricter environmental regulations on sulfur emissions. Reduction of sulfur emissions is typically achieved by deeper desulfurization of petroleum fuels which in turn requires additional hydrogen production (Crawford et al., 2002). A less capital intensive alternative to alleviate hydrogen shortage is to operate the catalytic reformer at higher severity. However, higher severity reforming increases the production of BTX aromatics which consequently affect the gasoline pool aromatics specification. Therefore, the BTX extraction process becomes a more viable alternative for the sake of aromatics recovery as well as maintaining the gasoline pool within specification (Crawford et al., 2002). The capital cost for the implementation of such a project would generally be lower as the BTX complex and refinery would share both process and utilities streams.

2.4.3 Fuel Gas Upgrade

Refinery fuel gas is generated from refinery processes and is mainly comprised of C_1/C_2 fractions and some hydrogen. Considerable amounts of light hydrocarbons are produced from the different conversion units in the refinery and are collected in the common fuel gas system. For instance, FCC off gas contains significant amounts of ethylene and propylene which can be extracted and processed as petrochemical feedstocks. A number of integrated U.S. and European refineries have recognized and capitalized on this opportunity by recovering these high value components (Swaty, 2002). This type of synergy requires proper planning and optimization between the petroleum refining and petrochemical complexes.

The other major component is hydrogen where it typically accounts for 50-80 % of the refinery fuel gas (Patel et al., 2003). This substantial amount of hydrogen is disposed to the fuel gas system from different sources in the refinery. The most significant source, however, is the catalytic reforming. Hydrogen recovery using economically attractive technologies is of a great benefit to both refineries and petrochemical systems especially with the increasing strict environmental regulations on fuels.

2.5 Production Planning under Uncertainty

In the current volatile market environment and the continuous change in customer requirements, the impact of uncertainties is a necessary consideration. As mentioned earlier, in production planning, sources of system uncertainties can be categorized as short-term or long-term depending on the extent of time horizon (Subrahmanyam et al., 1994). The short-term uncertainties mainly refer to operational variations, equipment failure, etc. Whereas, long-term uncertainty may include supply and demand rate variability and price fluctuations, on a longer time horizon (Shah, 1998). Technological uncertainty in the left-hand side coefficients which can be viewed in the context of production planning as the variation in process yields is another important uncertainty factor.

Different approaches have been devised to tackle optimization under uncertainty. These include stochastic optimization (two-stage, multistage) with recourse based on the seminal work of Dantzig (1955), chance-constrained optimization (Charnes & Cooper, 1959), fuzzy programming (Bellman & Zadeh, 1970), and design flexibility (Grossmann & Sargent, 1978). These early works on optimization under uncertainty have undergone substantial developments in both theory and algorithms (Sahinidis, 2004). In this section, we will

mainly concentrate on stochastic, chance-constrained (probabilistic) optimization, and robust optimization. For additional details and information, the interested reader is invited to pursue references such as Dempster (1980), Sahinidis (2004) and the recent textbooks of Kall and Wallace (1994) and Ruszczyński and Shapiro (2003).

2.5.1 Stochastic Programming

In this discussion we will explain the two-stage stochastic programming model. In a standard two-stage stochastic programming model, decision variables are divided into two groups; namely, first stage and second stage variables (Kall & Wallace, 1994). First stage variables are decided before the actual realization of the random parameters. Once the uncertain events have unfolded, further design or operational adjustments can be made through values of the second-stage or alternatively called recourse variables at a particular cost. This concept of recourse has had many applications to linear, integer, and non-linear programming (Sahinidis, 2004).

A standard formulation of the two-stage stochastic linear program is (Ruszczyński & Shapiro, 2003):

$$\begin{aligned} &Min_x \;\; c^T x + \mathrm{E}[Q(x,\xi(\omega))] \\ &s.t. \quad Ax = b, x \geq 0 \end{aligned} \tag{2.1}$$

where $Q(x,\xi(\omega))$ is the optimal value of the second stage problem:

$$\begin{aligned} &Min_x \;\; q^T y \\ &s.t. \quad Tx + Wy = h, y \geq 0 \end{aligned} \tag{2.2}$$

where x and y are vectors of the first and second stage decision variables, respectively. The second stage problem depends on the data $\xi = (q, h, T, W)$ where any or all elements can be random. The expectation in (2.1) is with respect to the probability distribution of $\xi(\omega)$. Matrices T and W are called technological and recourse matrices, respectively. The second stage problem (2.2) can be considered as penalty for the violation of the constraint Tx=h.

There are two different ways of representing uncertainty (Gupta and Maranas, 2000). The first approach is the continuous probability distribution where numerical integration is employed over the random continuous probability space. This approach maintains the model size but on the other hand introduces nonlinearities and computational difficulties to the problem. The other approach is the scenario-based approach where the random space is considered as discrete events. The main disadvantage of this approach is the substantial increase in computational requirements with increasing the number of uncertain parameters (Shah, 1998). The discrete distribution with a finite number K of possible outcomes (scenarios) $\xi_k = (q_k, h_k, T_k, W_k)$ corresponds to the probability p_k. Hence, equations (2.1) and (2.2) can be written as a deterministic equivalent problem and represented as follows (Ruszczyński & Shapiro, 2003):

$$
\begin{aligned}
& Min_{x, y_1, \ldots y_k} \quad c^T x + \sum_{k=1}^{K} p_k q_k^T y_k \\
& s.t. \qquad Ax = b \\
& \qquad\quad T_k x + W_k y_k = h_k \qquad k = 1, \ldots, K \\
& \qquad\quad x \geq 0, y_k \geq 0 \qquad\quad k = 1, \ldots, K
\end{aligned}
\tag{2.3}
$$

In this thesis, due to the complexity of numerical integration and the exponential increase in sample size with the increase of the random variables, we will employ an approximation

scheme know as the Sample Average Approximation (SAA) method, also as stochastic counterpart. The Sample Average Approximation problem can be written as (Verweij et al. 2003):

$$v_N = \min_{x \in X} c^T x + \frac{1}{N} \sum_{k \in N} Q(x, \xi^k) \tag{2.4}$$

It approximates the expectation of the stochastic formulation (usually called the "true" problem) and can be solved using deterministic algorithms. The SAA method was used among others by Shapiro and Homemde-Mello (1998), Mark et al. (1999), Linderoth et al. (2002) for stochastic linear problems, Kleywegt et al. (2001), Verweij et al. (2003) for stochastic integer problems, and Wei and Realff (2004), Goyal and Ierapetritou (2007) for MINLP problems. Further details of this approximation scheme will be discussed in Chapter 4.

2.5.2 Chance Constrained Programming

The philosophy of the previous methods to stochastic programming was to ensure feasibility of the problem through the second-stage problem at a certain penalty cost. In the chance-constrained approach, some of the problem constraints are expressed probabilistically, requiring their satisfaction with a probability greater than a desired level (Kall & Wallace, 1994). This approach is particularly useful when the cost and benefits of second-stage decisions are difficult to assess as the use of second-stage or recourse actions is avoided. These intangible components include loss of goodwill, cost of off-specification products and outsourcing of production (Wenkai et al., 2004).

For a typical linear programming model:

$$Min_x \ c^T x \quad s.t. \ Ax \geq b, x \geq 0 \tag{2.5}$$

Assume that there is uncertainty in the matrix A (left-hand-side coefficient) and in the right-hand-side vector b and the above constraint must be satisfied with a probability $p \in (0,1)$. Then the probabilistic model can be expressed as follows (Ruszczyński & Shapiro, 2003):

$$Min_x \ c^T x \quad s.t. \ P(Ax \geq b) \geq p, x \geq 0 \tag{2.6}$$

If we consider a single constraint, for the sake of simplicity, then the above becomes $P(a^t x \geq b) \geq p$. Furthermore, assume the randomness is only in the right-hand-side with a distribution of *F*. When $F(\beta) = p$, then constraint can be written as $F(a^t x) \geq p \rightarrow a^t x \geq \beta$. In this case, the model yields a standard linear program (Sahinidis, 2004).

Programming under probabilistic constraints was first demonstrated in the seminal work by Charnes and Cooper (1959). Since then many applications were developed for different sectors including capacity design in power networks (Bloom, 1988), environmental (Pintér, 1991), aviation (Kibzun & Kan, 1996) and refining problems (Wenkai et al., 2004).

2.5.3 Robust Optimization

The stochastic model with recourse in the previous section takes a decision merely based on first-stage and expected second-stage costs leading to an assumption that the decision-maker is risk-neutral (Sahinidis, 2004). In order to capture the concept of risk in stochastic programming, Mulvey et al. (1995) proposed the following amendment to the objective function:

$$Min_{x,y} \; c^T x + \mathrm{E}[Q(x,\xi(\omega))] + \lambda f(\omega, y) \tag{2.7}$$

where f is a measure of variability of the second-stage costs and λ is a non-negative scalar representing risk tolerance which is usually decided by the modeler. This representation is referred to as mean-risk model (Ahmed et al., 2007). This formulation follows the representation of the Markowitz mean–variance (MV) model (Markowitz, 1952). The variability measure can be modeled as variance, mean-absolute deviation or financial measures of Value-at-Risk (VaR) and Conditional Value-at-Risk (CVaR).

In this thesis, we use the representation of risk management using variance as a risk measure following the proposed method by Mulvey et al. (1995) in which they referred to this approach as robust stochastic programming. They defined two types of robustness: 1) solution robustness referring to the optimal model solution when it remains close to optimal for any scenario realization, and 2) model robustness representing an optimal solution when it is almost feasible for any scenario realization.

The context of solution and model robustness in this thesis will be explained in the coming chapters depending on the uncertainty variables considered in the multisite refining planning, petrochemical planning, and multisite refinery and petrochemical integration problems.

Chapter 3

Optimization of Multisite Refinery Network: Integration and Coordination

3.1 Introduction

With the current situation of high crude oil prices and the everlasting pressure to reduce prices of final petroleum products, refiners are faced with a very challenging situation. This nature of petroleum economic environment is a pressing motive for refineries to operate at an optimal level and continue to seek opportunities to increase their profit margin. This requires appropriate high level decision-making to utilize all available resources not only on a single facility scale, but in a more comprehensive outlook of an enterprise-wide scale. Such approach provides an enhanced coordination and objectives alliance towards achieving a global optimal production strategy (Chopra & Meindl, 2004). The benefits projected from the coordination of multiple sites are not only in terms of expenses but also in terms of market effectiveness and responsiveness (Shah, 1998). Most of the time, there will be some necessity for a degree of independent management at each operating entity. However, the need for a coordinated response and the desire to minimize costs, imply that the various entities should be treated as parts of one large production system (Wilkinson, 1996). Planning for this system should be carried out centrally, allowing proper interactions between all operating facilities and consequently an efficient utilization of available resources. The

understanding of such benefits has attracted a lot of research in the areas of strategic planning in general and supply chain design and coordination in particular.

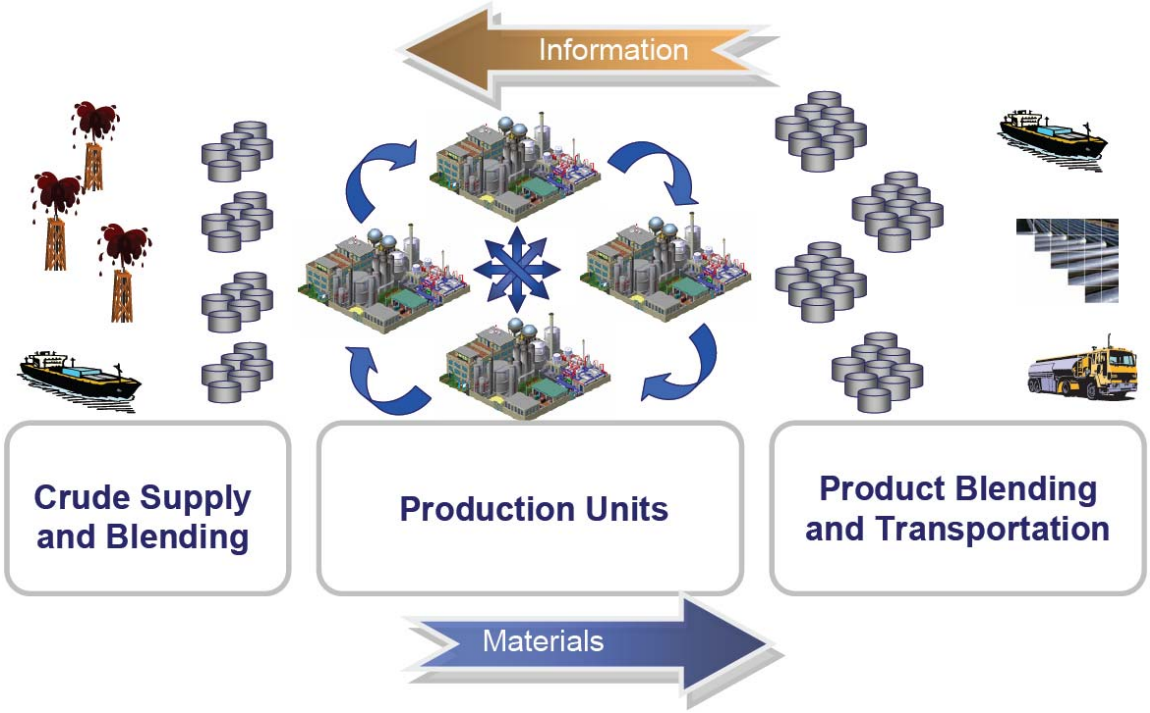

Figure 3.1 Refinery supply chain with process network integration.

The objective of this work is to develop a methodology that can be applied for designing and analyzing process integration networks and production capacity expansions in a multiple refineries complex using different feedstocks combination alternatives, Figure 3.1. The integration strategy will allow the optimal coordination of the entire operating system through exchange of intermediate and product streams as well as the efficient utilization of available resources in the different operating sites. The integration of utility streams between the different sites is beyond the scope of this study, as we mainly address process streams. The proposed model is formulated as a mixed-integer linear programming (MILP) problem that minimizes an annualized operating and capital cost of the system. The application of the proposed methodology to achieve an integration and coordination strategy to the oil refining

industry adds more complications and challenges. This is due to the fact that refining is one of the most complex chemical industries which comprises complicated processes and various configurations and structural alternatives. Although the MILP model was developed and applied to the refining industry in this study, it can be extended to any network of chemical processes. Since the decisions in this study are of a long-term planning horizon, a linear model formulation is adequate to capture the required details of refinery processes (Zhang & Zhu, 2006). All capital cost investments were discounted over a time horizon in order to support a net present worth analysis.

Bok et al. (2000) explained a classification of chemical process networks and characterized them as either dedicated or flexible processes. Dedicated processes operate at one mode and for high volume products whereas flexible processes operate at different modes and produce different products at different times. In our formulation, we account for different operating modes. This should not be confused with flexible processes as the different modes in this study represent different product yields and do not require any set up costs or changeover times.

The remainder of Chapter 3 is organized as follows. In the following section we will provide a literature review on process expansions and multisite planning and coordination studies in the chemical process industry. Then we will explain the problem statement and proposed model formulation in section 3.3 and 3.4, respectively. In section 3.5, we will illustrate the performance of the model through various industrial-scale refinery examples and scenarios. The Chapter ends with some concluding remarks in section 3.6.

3.2 Literature Review

There has been quite a large stream of research concerned with capacity expansions and retrofit problems in the chemical and operations research literature. In this section, however, we will concentrate on expansion and strategic multisite planning studies. Single site short-term and mid-term planning and scheduling studies are beyond the scope of this thesis and the interested reader is referred to the work by Bodington and Baker (1990), Pinto and Moro (2000), and Kallrath (2005).

One of the early attempts in the operations research literature that considered multiple echelons and sites seems to be that of Williams (1981). Williams investigated different heuristic techniques of varying sophistication for production-distribution scheduling. Although he used simplifying assumptions, his work is one of the early attempts in the operations research literature in the use of coordinated planning across multiple echelons and sites. In the process systems engineering community, large scale multisite planning and coordination models had a bigger share just recently.

Many earlier studies tackled different expansion problems in the chemical industry including the NLP formulation by Himmelblau and Bickel (1980) and multiperiod MILP model by Grossmann and Santibanez (1980) and the recursive MILP model by Jimenez and Rudd (1987). A common drawback among these studies was their limitation of problem size due to computational burden. Other papers on capacity expansions can be found in Roberts (1964), Manne (1967) and Florian et al. (1980) where discussions of how relevant these problems are to the industry are also provided. More recently, Sahinidis et al. (1989) developed a multiperiod MILP model for strategic planning in terms of selection and

expansion of processes given forecasted demands and prices. In their study, they investigated several solution strategies to reduce model computational burden. The strategies included branch and bound, integer cuts, cutting planes, Benders decomposition and other heuristics. This model was later reformulated by Sahinidis and Grossmann (1991a, 1992) by identifying a lot sizing problem structure within the long-range problem formulation. The new reformulation improved the solution efficiency through tighter linear relaxation to the MILP model. The model was expanded to include continuous and batch flexible and dedicated processes (Sahinidis & Grossmann, 1991b). Along the same lines, Norton and Grossmann (1994) extended the work by Sahinidis et al. (1989) to account for dedicated and flexible processes in terms of feedstocks, products and the combination of continuous and batch processes. They illustrated their example on a petrochemical complex.

Wilkinson et al. (1996) proposed an approach that integrates production and distribution in multisite facilities using the resource task network representation proposed by Pantelides (1994). They applied this technique to an industrial case across a whole continent that involved the production and distribution planning among different factories and markets. In a similar problem, McDonald and Karimi (1997) studied multiple semicontinuous facilities in a number of geographically distributed customers. The aim was to find an optimal allocation of recourses to tasks to meet a certain demand over a time horizon. They included a number of additional supply chain type constraints such as single sourcing, internal sourcing, and transportation times.

Iyer and Grossmann (1998) revisited the work by Sahinidis et al. (1989) and used a bilevel decomposition approach to reduce the computational complexity of the problem with the objective of solving larger scenarios. In a similar effort, Bok et al. (2000) extended the

work by Norton and Grossmann (1994) to incorporate operational decisions over a short term horizon such as inventory profile, changeover cost, and intermittent supplies over multiple operating sites. They also used a bilevel decomposition approach to reduce computational time and illustrated their approach on several examples dealing with a petrochemical complex. Their model addressed short term operating decisions and provided no insight on designing or retrofitting the process network.

Shah (1998) presented a review of the production planning and scheduling in single and multiple facilities. He pointed out that multisite problems have received little attention and are potential candidates for future research. Bunch et al. (1998) developed MILP model to find the lowest cost alternative among existing geographically distributed pharmaceutical facilities to satisfy a given demand. The model was used to find optimal assignment of products to facilities and production quantities over a time horizon. They used a commercial scheduling software (VirtECS) for both problem representation and solution. In their study, there was no clear underlying structure of the problem or a systematic approach for the model formulation. Furthermore, the solution approach did not guarantee optimality.

Timpe and Kallrath (2000) developed a multi-period MILP model for a complete supply chain management of a multisite production network. The problem was formulated and applied to the food industry. The model concentrated on the coordination of the different echelons of the food supply chain and did not cover developing an integration scheme for the multiste facilities. Swaty (2002) studied the possibility of integrating a refinery and an ethylene plant through the exchange of process intermediate streams. The analysis was based on a linear programming (LP) model for each plant and profit marginal analysis of possible intermediate plant exchange. The study was implemented on a real life application in

western Japan. Jackson and Grossmann (2003) proposed a multiperiod nonlinear programming model for production planning and distribution over multisite facilities. They used a temporal decomposition technique to reduce the scale of the problem.

Lasschuit and Thijssen (2004) pointed out the importance of developing integrated supply chain planning models on both strategic and tactical levels in the petroleum and chemical industry. They also stressed on the issues that need to be accounted for when formulating these models. Neiro and Pinto (2004) proposed a general framework for modeling operational planning of the petroleum supply chain. They developed MINLP model for the planning of multiple existing refineries, terminals and pipeline networks. Decisions included the selection of oil types and scheduling plan to the refineries subject to quality constraints as well as processing units, operating variables, product distribution, and inventory management. The model was applied to an industrial case in Brazil. Due to the high computational burden, the model was only solved for two time periods. The authors suggested that decomposition methods should be applied to yield a smaller MINLP or MILP model. Their approach did not consider the design problem of a network of operating facilities as their formulation addressed only operational type decisions.

Ryu and Pistikopoulos (2005) presented MILP model for the design of enterprise-wide supply chains in the chemical industry. They investigated three different operating policies, namely, competition, cooperation and coordination. Their model was based on the assumption that plants will always have much larger capacities than demand. Furthermore, their work was mainly concerned with optimizing the operating policies among the different echelons of the supply chain and did not account for designing an integration policy between the multisite production facilities.

Khogeer (2005) developed a LP model for multiple refinery coordination. He developed different scenarios to experiment with the effect of catastrophic failure and different environmental regulation changes on the refineries performance. This work was developed using commercial planning software (Aspen PIMS). In his study, there was no model representation of the refineries systems or clear simultaneous representation of optimization objective functions. Such an approach deprives the study from its generalities and limits the scope to a narrow application. Furthermore, no process integration or capacity expansions were considered.

Another stream of research tackled modeling uncertainty in capacity expansion and supply chain studies in the process industry. Ierapetritou and Pistikopoulos (1994) developed a two-stage stochastic programming model for short to long-term planning problems. They proposed a decomposition method based on the generalized Benders decomposition algorithm where they used a Gaussian quadrature to estimate the expectation of the objective function. Liu and Sahinidis (1995; 1996; 1997) studied design uncertainty in process expansion through sensitivity analysis, stochastic programming and fuzzy programming, respectively. In their stochastic model, they used Monte Carlo sampling to calculate the expected objective function values. Their comparison over the different methodology of including uncertainty was in favor of stochastic models when random parameters distributions are not available.

On a larger scale, Tsiakis et al. (2001) developed a supply chain design for multiple markets and plants of steady-state continuous processes. Similarly, Ryu et al. (2004) presented a bilevel framework for planning an enterprise-wide network under uncertainty of some product demands plant and warehouse capacities as well as resource availability. They

considered the hierarchy of the supply chain and allowed for optimizing different levels of the chain individually.

The above discussion clearly points out the importance of multisite planning and indicates that such a problem is attracting a great deal of interest as the realizations of the coordinated benefits became more vivid. However, to the best of our knowledge, no previous work has tackled developing a general framework for designing a network between multiple refineries in terms of material exchange. The aim of this study is to provide a methodology of the design of an integration and coordination policy of multiple refineries to explore potential synergies and efficient utilization of resources across an enterprise or multiple enterprises. The expansions of the facilities and the construction of the integration network are assumed to be implemented simultaneously in a single time horizon in order to minimize future process interruptions. Although our discussion will consistently refer to a network of refineries, the methodology that we will present can be readily extended to other chemical process networks.

3.3 Problem Statement

The optimization of refining processes involves a broad range of aspects varying from economical analysis and strategic expansions to crude oil selection, process levels targets, operating modes, etc. The focus of this study is the development of a methodology for designing an integrated network and production expansion across multiple refineries as well as the establishment of an operating policy that sets feedstock combinations, process levels and operating mode preferences to satisfy a given demand. Such integration will provide

appropriate means for improving the coordination across the whole network production system.

The general integration problem can be defined as:

A set of products $cfr \in CFR$ to be produced at multiple refinery sites $i \in I$ is given. Each refinery consists of different production units $m \in M_{Ref}$ that can operate at different operating modes $p \in P$. An optimal feedstock from different available crudes $cr \in CR$ is desired. Furthermore, the process network across the multiple refineries is connected in a finite number of ways and an integration superstructure is defined. Market product prices, operating cost at each refinery, as well as product demands are assumed to be known.

The problem consists of determining the optimal integration for the overall network and associated coordination strategies across the refinery facilities as well as establishing an optimal overall production and determining the operating levels for each refinery site. The objective is to minimize the annualized cost over a given time horizon by improving the coordination and utilization of excess capacities in each facility. Expansion requirements to improve production flexibility and reliability are also considered.

For all refinery processes within the network we assume that all material balances are expressed in terms of linear yield vectors. Even though this might sound to be restrictive as most if not all refinery processes are inherently nonlinear, this practice is commonly applied in the petroleum refining business. Moreover, the decisions in this study are of a strategic level in which such linear formulation is adequate to address the required level of details involved at this stage. It is also assumed that processes have fixed capacities and the

operating cost of each process and production mode is proportional to the process inlet flow. In the case of product blending, quality blending indices are used to maintain model linearity. Blending indices tables and graphs can often be found in petroleum refining books such as Gary and Handwerk (1994) or can be proprietarily developed by refining companies for their own use. It is also assumed that all products that are in excess of the local demand can be exported to a global market. Piping and pumping installation costs to transport intermediate streams as well as the operating costs of the new system were lumped into one fixed-charge cost. All costs are discounted over a 20 years time horizon and with an interest rate of 7%. No inventories will be considered since the model is addressing strategic decisions which usually cover a long period of time. We also assume perfect mixing and that the properties of each crude type are decided by specific key components. Properties of the oil mixture, such as viscosity, do not affect the strategic decisions of network design immensely and are therefore not considered in the model. Such considerations renders the model unnecessary complicated and are even tolerable on studies of operational planning and scheduling level (Lee et al., 1996; Jia & Ierapetritou, 2003, 2004).

3.4 Model Formulation

The model is formulated based on the State Equipment Network (SEN) representation (Yeomans & Grossmann, 1999). The general characterization of this representation includes three elements: state, task and equipment. A State includes all streams in a process and is characterized by either quantitative or qualitative attributes or both. The quantitative characteristics include flowrate, temperature and pressure whereas the qualitative characteristics include other attributes such as the phase(s) of the streams. A task, on the other hand, represents the physical and chemical transformations that occur between

consecutive states. Equipment provides the physical devices that execute a given task (e.g. reactor, absorber, heat exchanger).

The state equipment network (SEN) allows for two types of task to equipment assignment: The first type is one task-one equipment (OTOE) assignment where tasks are assigned to equipment a priori. This type of assignment yields an identical representation to the state task network (STN) by Kondili et al. (1993). The second type is the variable task equipment assignment where the actual assignment of tasks to equipment is considered as part of the optimization problem. The use of this representation provides a consistent modeling strategy and an explicit handling of units that operate under different modes, which is common in the refining industry.

In treating stream mixing, the mixing device was defined as part of the designated refinery operation itself. This approach was also undertaken by Zhang and Zhu (2006). Therefore the only mixers considered are where the final blending takes place. This approach distinguishes the contribution of each feedstock to the final product. With this type of formulation, all variables and attributes of intermediate streams will depend on the crude type.

The problem is formulated as an MILP model where binary variables are used for designing the process integration network between the refineries and deciding on the production unit expansion alternatives. Linearity in the model was achieved by defining component flows instead of individual flows and associated fractions. The planning problem formulation is as follows.

3.4.1 Material Balance

The material streams, states, and their balances are divided into four categories; namely; raw materials, intermediates, products, and fuel system. All material balances are carried out on a mass basis. However, volumetric flowrates are used in the case where quality attributes of some streams only blend by volume.

Constraint (3.1) below illustrates the refinery raw materials balance in which throughput to each refinery crude distillation units $p \in P'$ at plant $i \in I$ from each crude type $cr \in CR$ is equal to the available supply $S^{Ref}_{cr,i}$.

$$z_{cr,p,i} = S^{Ref}_{cr,i} \qquad \forall \ cr \in CR,\ i \in I \quad \text{where} \quad p \in P' = \{\text{Set of CDU processes} \ \forall \ \text{plant i}\} \tag{3.1}$$

The intermediate material balances within and across the refineries can be expressed as shown in constraint (3.2). The coefficient $\alpha_{cr,cir,i,p}$ can assume either a positive sign if it is an input to a unit or a negative sign if it is an output from a unit. The multirefinery integration matrix $\xi_{cr,cir,i,p,i'}$ accounts for all possible alternatives of connecting intermediate streams $cir \in CIR$ of crude $cr \in CR$ from refinery $i \in I$ to process $p \in P$ in plant $i' \in I'$. Variable $xi^{Ref}_{cr,cir,i,p,i'}$ represents the transshipment flowrate of crude $cr \in CR$, of intermediate $cir \in CIR$ from plant $i \in I$ to process $p \in P$ at plant $i' \in I$. The process network integration superstructure that constitutes all possible configuration structures can be defined a priori through suitable engineering and process analysis of all possible intermediate streams exchange.

$$\sum_{p\in P}\alpha_{cr,cir,i,p}\ z_{cr,p,i}+\sum_{i'\in I}\sum_{p\in P}\xi_{cr,cir,i',p,i}\ xi^{Ref}_{cr,cir,i',p,i}$$
$$-\sum_{i'\in I}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'}-\sum_{cfr\in CFR}w_{cr,cir,cfr,i}-\sum_{rf\in FUEL}w_{cr,cir,rf,i}=0 \qquad \forall \begin{array}{l} cr\in CR,\\ cir\in CIR,\\ i'\,\&\,i\in I\\ \text{where } i\neq i'\end{array} \tag{3.2}$$

The material balance of final products in each refinery is expressed as the difference between flowrates from intermediate steams $w_{cr,cir,cfr,i}$ for each $cir \in CIR$ that contribute to the final product pool and intermediate streams that contribute to the fuel system $w_{cr,cfr,rf,i}$ for each $rf \in FUEL$ as shown in constraint (3.3). In constraint (3.4) we convert the mass flowrate to volumetric flowrate by dividing it by the specific gravity $sg_{cr,cir}$ of each crude type $cr \in CR$ and intermediate stream $cir \in CB$. This is done as some quality attributes blend only by volume in the products blending pools.

$$\sum_{cr\in CR}\sum_{cir\in CB}w_{cr,cir,cfr,i}-\sum_{cr\in CR}\sum_{rf\in FUEL}w_{cr,cfr,rf,i}=x^{Ref}_{cfr,i} \qquad \forall \begin{array}{l} cfr\in CFR,\\ i\in I\end{array} \tag{3.3}$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}}=xv^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ i\in I \tag{3.4}$$

Constraint (3.5) is the fuel system material balance where the term $cv_{rf,cir,i}$ represents the caloric value equivalent for each intermediate $cir \in CB$ used in the fuel system at plant $i \in I$. The fuel production system can either consist of a single or combination of intermediates $w_{cr,cir,rf,i}$ and products $w_{cr,cfr,rf,i}$. The matrix $\beta_{cr,rf,i,p}$ corresponds to the consumption of each processing unit $p \in P$ at plant $i \in I$ as a percentage of unit throughput.

$$\sum_{cir\in FUEL}cv_{rf,cir,i}\ w_{cr,cir,rf,i}+\sum_{cfr\in FUEL}w_{cr,cfr,rf,i}-\sum_{p\in P}\beta_{cr,rf,i,p}\ z_{cr,p,i}=0 \qquad \forall \begin{array}{l} cr\in CR,\\ rf\in FUEL,\\ i\in I\end{array} \tag{3.5}$$

3.4.2 Product Quality

In general, the quality of a blend is composed of multiple components and is given by the following blending rule (Favennec et al., 2001):

$$Q = \frac{\sum q_i X_i}{\sum X_i}$$

where Q is the quality attribute of the blend, X_i is the quantity of each component in the blend, and q_i is the quality attribute of each blending component. However, when dealing with a big variety of blended products as in the case of refining, we need to distinguish between attributes or components that blend by weight such as sulfur content and others that blend by volume such as vapor pressure and octane number of gasoline. Furthermore, it is important to replace certain quality measurements such as viscosity values with certain blending indices in order to maintain model linearity. Blending indices tables and graphs can be found in petroleum refining books such as Gary and Handwerk (1994) or can be proprietarily developed by refining companies for their own use.

Constraints (3.6) and (3.7), respectively, express the lower and upper bound on quality constraints for all products that either blend by mass $q \in Q_w$ or by volume $q \in Q_v$.

$$\sum_{cr \in CR} \sum_{cir \in CB} \left(att_{cr,cir,q \in Qv} \frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} + att_{cr,cir,q \in Qw} \left[w_{cr,cir,cfr,i} - \sum_{rf \in FUEL} w_{cr,cfr,rf,i} \right] \right) \geq q^{L}_{cfr,q \in Qv} \; xv^{Ref}_{cfr,i} + q^{L}_{cfr,q \in Qw} \; x^{Ref}_{cfr,i} \qquad \begin{array}{l} \forall \\ cfr \in CFR, \\ q = \{Qw, Qv\}, \\ i \in I \end{array} \qquad (3.6)$$

$$\sum_{cr \in CR} \sum_{cir \in CB} \left(att_{cr,cir,q \in Qv} \frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} + att_{cr,cir,q \in Qw} \left[w_{cr,cir,cfr,i} - \sum_{rf \in FUEL} w_{cr,cfr,rf,i} \right] \right) \leq q^{U}_{cfr,q \in Qv} \; xv^{Ref}_{cfr,i} + q^{U}_{cfr,q \in Qw} \; x^{Ref}_{cfr,i} \qquad \begin{array}{l} \forall \\ cfr \in CFR, \\ q = \{Qw, Qv\}, \\ i \in I \end{array} \qquad (3.7)$$

3.4.3 Capacity Limitation and Expansion

Constraint (3.8) represents the maximum and minimum allowable flowrate to each processing unit. The coefficient $\gamma_{m,p}$ represents a zero-one matrix for the assignment of production unit $m \in M_{Ref}$ to process operating mode $p \in P$. As an example, the reformer is a production unit that can operate at high or low severity modes. The selection of the mode of operation will be considered as part of the optimization problem where variable task-equipment assignment (VTE) will be used. The term $AddC_{m,i,s}$ represents the additional expansion capacity for each production unit $m \in M_{Ref}$ at refinery $i \in I$ for a specific expansion size $s \in S$. Production systems expansion through the addition of new units requires detailed analysis and is usually quoted not only based on the unit flowrate but also on many other factors. For this reason, developing cost models of such expansions only as a function of the unit flowrate does not generally provide a good estimate. In our formulation, we only allowed the addition of predetermined capacities whose pricing can be acquired a priori through design companies' quotations. The integer variable $yexp^{Ref}_{m,i,s}$ represents the decision of expanding a production unit and it can take a value of one if the unit expansion is required or zero otherwise.

$$MinC_{m,i} \le \sum_{p \in P} \gamma_{m,p} \sum_{cr \in CR} z_{cr,p,i} \le MaxC_{m,i} + \sum_{s \in S} AddC_{m,i,s}\ yexp^{Ref}_{m,i,s} \quad \forall\ m \in M_{Ref}, i \in I \tag{3.8}$$

Constraint (3.9) sets an upper bound on intermediate streams flowrates between the different refineries. The integer variable $ypipe^{Ref}_{cir,i,i'}$ represents the decision of exchanging intermediate products between the refineries and takes on the value of one if the commodity is transferred from plant $i \in I$ to plant $i' \in I$ or zero otherwise, where $i \neq i'$. When an

intermediate stream is selected to be exchanged between two refineries, its flowrate must be below the transferring pipeline capacity $F^{U}_{cir,i,i'}$.

$$\sum_{cr\in CR}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'} \le F^{U}_{cir,i,i'}\ y_{pipe}{}^{Ref}_{cir,i,i'} \qquad \forall \begin{array}{l} cir \in CIR,\ i' \,\&\, i \in I \\ \text{where } i \neq i' \end{array} \tag{3.9}$$

3.4.4 Product Demand

Constraint (3.10) stipulates that the final products from each refinery $x^{Ref}_{cfr,i}$ less the amount exported $e^{Ref}_{cfr',i}$ for each exportable product $cfr' \in PEX$ from each plant $i \in I$ must satisfy the domestic demand $D_{Ref_{cfr}}$.

$$\sum_{i\in I}\left(x^{Ref}_{cfr,i} - e^{Ref}_{cfr',i}\right) \ge D_{Ref_{cfr}} \qquad \forall \begin{array}{l} cfr \ \&\ cfr' \\ \text{where} \quad cfr \in CFR,\ cfr' \in PEX \end{array} \tag{3.10}$$

3.4.5 Import Constraint

The imports or resources constraint (3.11) imposes upper and lower bounds on the available feedstock $cr \in CR$ to the refineries. The lower bound constraint might be useful in the cases where there are protocol agreements to exchange or supply crude oil between countries.

$$IM^{L}_{cr} \le \sum_{i\in I} S^{Ref}_{cr,i} \le IM^{U}_{cr} \qquad \forall\ cr \in CR \tag{3.11}$$

3.4.6 Objective Function

The objective function considered in this study is given by:

$$
\begin{aligned}
Min \quad & \sum_{cr \in CR} \sum_{i \in I} CrCost_{cr} \; S^{Ref}_{cr,i} \\
& + \sum_{p \in P} OpCost_{p} \sum_{cr \in CR} \sum_{i \in I} z_{cr,p,i} \\
& + \sum_{cir \in CIR} \sum_{i \in I} \sum_{i' \in I} InCost_{i,i'} \; ypipe^{Ref}_{cir,i,i'} \qquad \text{where } i \neq i' \\
& + \sum_{i \in I} \sum_{m \in M_{Ref}} \sum_{s \in S} InCost_{m,s} \; yexp^{Ref}_{m,i,s} \\
& - \sum_{cfr \in PEX} \sum_{i \in I} Pr^{Ref}_{cfr} \; e^{Ref}_{cfr,i}
\end{aligned}
\tag{3.12}
$$

The above objective represents a minimization of the annualized cost which comprises of crude oil cost, refineries operating cost, refineries intermediate exchange piping cost, production system expansion cost, and export revenue. The operating cost of each process is assumed to be proportional to the process inlet flow and is expressed on a yearly basis.

3.5 Illustrative Case Study

In this section, we present two examples with different scenarios. The first example illustrates the performance of the model on a single site total refinery planning problem where we compare the results of the model to an industrial scale study from Favennec et al. (2001). This example serves to validate our model and to make any necessary adjustments. The second example extends the scale of the model application to cover three complex refineries in which we demonstrate the different aspects of the model. The refineries considered are of large industrial-scale refineries and actually mimic a general set up of many areas around the world. The decisions in this example include the selection of crude blend combination, design of process integration network between the three refineries, and decisions on production units' expansion options and operating levels.

The modeling system GAMS (Brooke et al., 1996) was used for setting up the optimization models and the problems are solved by BDMLP 1.3 on a Pentium M processor 2.13 GHz.

3.5.1 Single Refinery Planning

Figure 3.2 provides a SEN representation of the refinery considered in this example. The planning horizon was set to one month in order to compare the model results to those of Favennec et al. (2001). As shown in Figure 3.2, the refinery uses two different feedstocks (e.g. Arabian light and Kuwait crudes) where the optimum blend is used to feed the atmospheric crude unit. The atmospheric crude unit separates crude oil into several fractions including LPG, naphtha, kerosene, gas oil and residues. The heavy residues are then sent to the vacuum unit where they are further separated into vacuum gas oil and vacuum residues. Depending on the production targets, different processing and treatment processes are applied to the crude fractions. In this example, the naphtha is further separated into heavy and light naphtha. Heavy naphtha is sent to the catalytic reformer unit to produce high octane reformates for gasoline blending and light naphtha is sent to light naphtha pool and to an isomerization unit to produce isomerate for gasoline blending too. The middle distillates are combined with other similar intermediate streams and sent for hydrotreating and then for blending to produce jet fuels and gas oils. Atmospheric and vacuum gas oils are further treated by catalytic cracking and in other cases by hydrocracking or both to increase the gasoline and distillate yields. In some refineries, vacuum residues are further treated using cooking and thermal processes to increase light products yields. The final products in

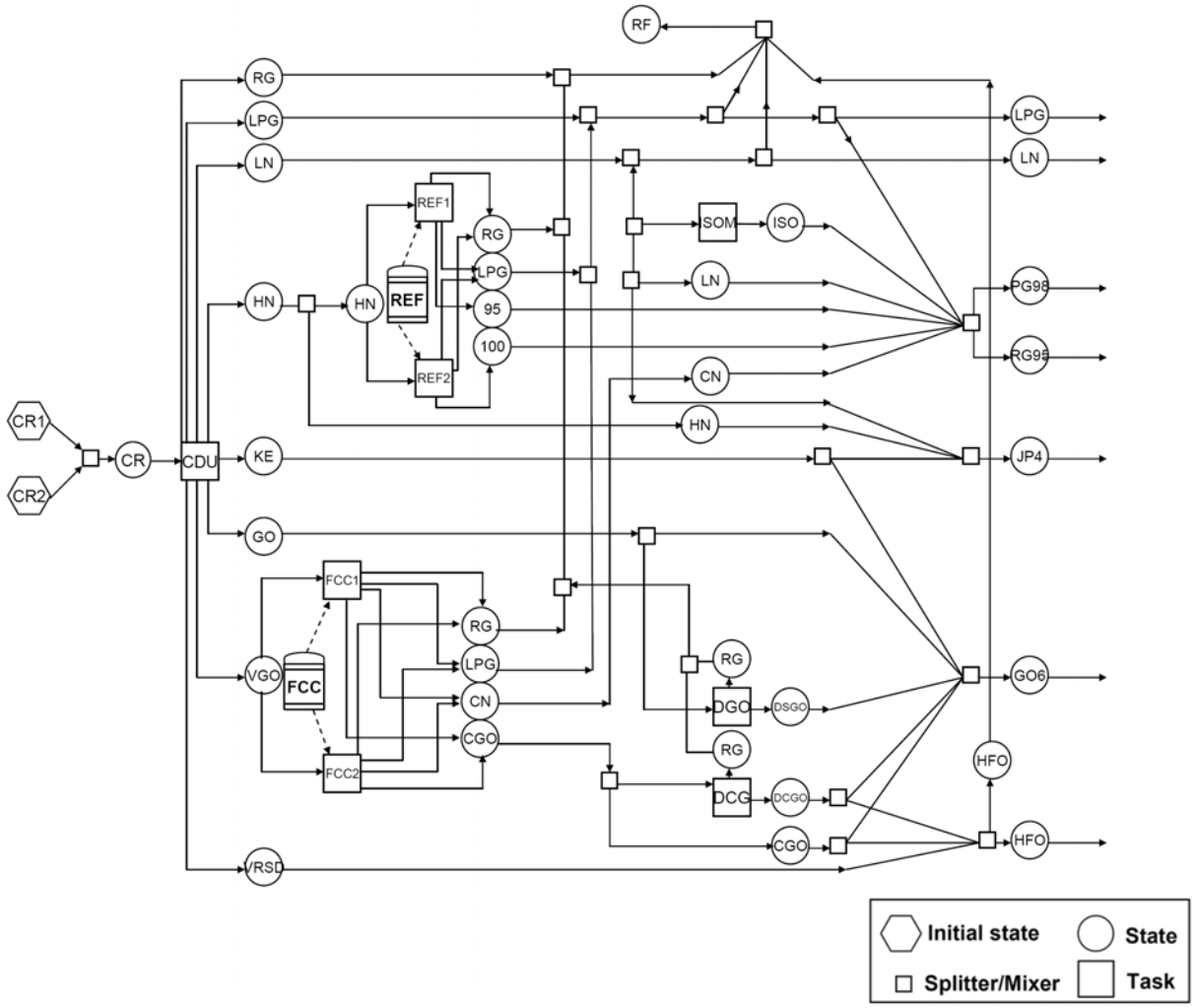

Figure 3.2 Refinery 1 layout using SEN representation.

this example consist of liquefied petroleum gas (LPG), light naphtha (LT), two grades of gasoline (PG98 and PG95), No.4 jet fuel (JP4), No.6 gas oil (GO6), and heating fuel oil (HFO). The major capacity limitations as well as availability constraints are shown in Table 3.1.

We slightly adjusted our model to allow for spot market buying and selling of heavy naphtha, vacuum gas oil and all products in order to demonstrate actual total site refinery planning and compare our results to Favennec et al. (2001). The model results and a comparison are shown in Table 3.2.

This example illustrates the capability and flexibility of our formulation to capture the details of a tactical or a medium-term planning horizon of one month. There are some minor differences in the results. This is because we were not able to access the detailed model used in their study and hence were not able to match their assumptions.

Table 3.1 Major refinery capacity constraints for single refinery planning

	Lower limit 1000 ton/month	**Higher limit 1000 ton/month**
Production Capacity		
Distillation	-	700
Reformer		
95 severity	2	-
Total	-	60
Isomerization	-	15
Fluid catalytic cracker	-	135
Total Desulfurization	-	150
Crude availability		
Crude 1	-	400
Crude 2	260	-

However, our proposed modeling methodology is of great benefits to refiners as they can align their long and medium plans through a common purpose model.

Table 3.2 Model results and comparison of single refinery planning

Process variables		Results (1000 ton/month)	
		Case Study	**Proposed model**
Crude oil supply	Crude 1	278.6	268.1
	Crude 2	260	260
	Total	538.6	528.1
Production levels	Crude	538.6	528.1
	Reformer 95	2	2
	Reformer 100	57.72	58.00
	Isomerization	11.72	11.63
	FCC gasoline mode	0	0
	FCC gas oil mode	130.5	128.4
	Des Gas oil	119.9	118.2
	Des cycle gas oil	23.8	23.0
Intermediate import	Heavy naphtha	7.38	8.62
Final product import	GO6	0	1
Exports	PG95	12.78	13.6
	JP4	5	0
Total cost ($/month)		90177	91970

3.5.2 Multisite Refinery Planning

In this example, we extend the scale of the case study to cover strategic planning for three complex refineries by which we demonstrate the performance of our model under different considerations. The three refineries considered represent industrial-scale size refineries and an actual configuration that can be found in may industrial sites around the world. See Figure 3.3 and Figure 3.4 for the second and third refinery layouts, respectively. These are in addition to the refinery case study of the single refinery planning in section 3.5.1. The three refineries are assumed to be in one industrial area, which is a common situation in many locations around the world. The refineries are coordinated through a main headquarter, centralized planning is assumed, and feedstock supply is shared. The final products of the three refineries consist of liquefied petroleum gas (LPG), light naphtha (LT), two grades of

gasoline (PG98 and PG95), No. 4 jet fuel (JP4), military jet fuel (ATKP), No.6 gas oil (GO6), diesel fuel (Diesel), heating fuel oil (HFO), and petroleum coke (coke). We will now consider several practical scenarios to demonstrate the advantage of the proposed integration model and its robustness under different considerations.

Scenario-1: single feedstock, multiple refineries with no integration. In this scenario, the three refineries are using a single feedstock type, Arabian Light, and operate centrally with no network integration alternatives. The major model constraints and results are shown in Table 3.3 and Table 3.4, respectively. The three refineries collaborate to satisfy a given local market demand where the model provides the production and blending level targets for the individual sites. Products that exceeded local market demand are either sold in the spot market or exported. The annual production cost across the facilities was found to be $7,118,000.

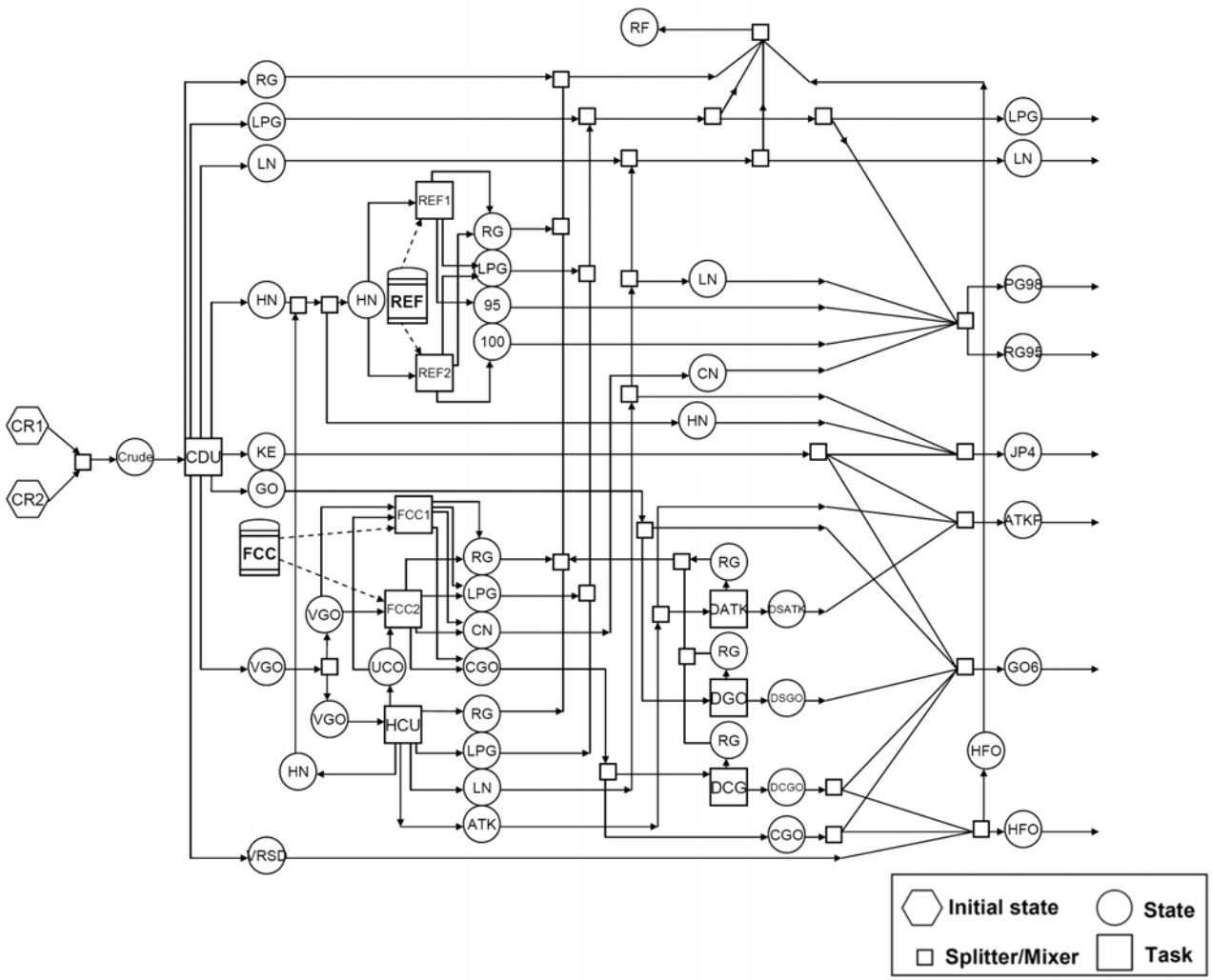

Figure 3.3 Refinery 2 layout using SEN representation.

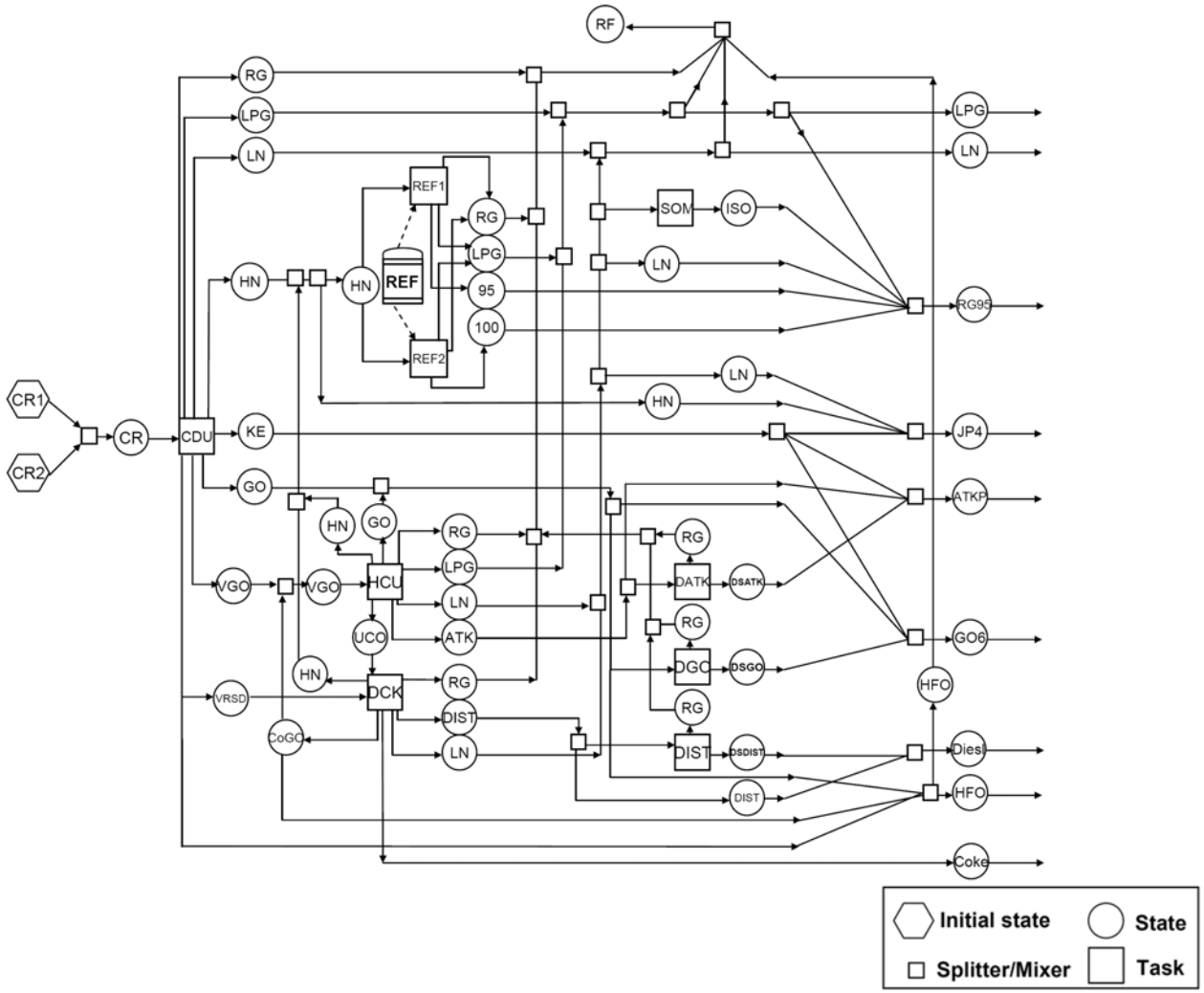

Figure 3.4 Refinery 3 layout using SEN representation.

Table 3.3 Major refineries capacity constraints for multisite refinery planning , Scenario-1&2

	Higher limit (1000 ton/yr)		
Production Capacity	R1	R2	R3
Distillation	4500	12000	9900
Reforming	1000	2000	1800
Isomerization	200	-	450
Fluid catalytic cracker	1700	1700	-
Hydrocracker	-	2000	2500
Delayed coker	-	-	2200
Des gas oil	1900	3000	2400
Des cycle gas oil	200	750	-
Des ATK	-	1200	1680
Des Distillates	-	-	700
Crude availability			
Crude 1		31200	
Crude 2		-	
Local Demand			
LPG		432	
LN		312	
PG98		540	
PG95		4440	
JP4		2340	
GO6		4920	
ATK		1800	
HFO		200	
Diesel		480	
Coke		300	

Scenario-2: single feedstock, multiple refineries with integration. In this scenario, we allowed the design of an integration network between the three refineries using the same set of constraints in Scenario-1. The cost parameters for pipelines installation were calculated as cost per distance between the refineries, and then multiplied by the required pipe length in order to connect any two refineries. The pipeline diameters considered in all cases was 8 inches.

Table 3.4 Model results of multisite refinery planning; Scenario-1

Process variables		Results (1000 ton/yr)		
		R1	**R2**	**R3**
Crude oil supply	Crude 1	4500	12000	9900
	Crude 2	-	-	-
	Total	4500	12000	9900
Production levels	Crude unit	4500	12000	9900
	Reformer 95	163.0	250.0	502.2
	Reformer 100	410.1	1574.6	1239.5
	Isomerization	140.3	-	450
	FCC gasoline mode	954	899.3	-
	FCC gas oil mode	-	-	-
	Hydrocracker	-	1740.4	2098.8
	Delayed coker	-	-	1402.4
	Des Gas oil	1395	2753.9	2383.8
	Des cycle gas oil	200	401.1	-
	Des ATK	-	1200	1447.1
	Des Distillates	-	-	338
Exports	PG95		214.3	
	JP4		1427	
	GO6		3540.1	
	HFO		1917.4	
	ATK		1508	
	Coke		176.8	
	Diesel		2.40	
Total cost ($/yr)			7,118,000	

As shown from this scenario results in Table 3.5, by allowing the design of an optimal integration network between the refineries, we were able to achieve annual savings exceeding $ 230,000. The savings will increase as the number of plants, production units and integration alternatives across the enterprise increase. However, benefits are not limited to reducing cost, but also include improved flexibility and sustainability of production as well as proper utilization and allocation of resources among the refineries network. As an example, diesel production in the first scenario (no integration) was barely satisfying local demand of 480,000 tones/year and only 2400 tones/year were left for export. With such a thin production margin, the plant did not have enough flexibility to face variations in diesel

demand. In scenario 2, however, the production margin of diesel increased from 2400 to 320,600 tones/year. The benefits were in terms of increasing exports and hence profit and also as gaining more diesel production flexibility to meet any variations in local market demand.

Table 3.5 Model results of multisite refinery planning; Scenario-2

Process variables				**Results (1000 ton/yr)**		
				R1	**R2**	**R3**
Crude oil supply	Crude 1			4500	12000	9900
	Crude 2			-	-	-
	Total			4500	12000	9900
Production levels	Crude unit			4500	12000	9900
	Reformer 95			-	-	887.2
	Reformer 100			573.1	2000	686.9
	Isomerization			140.3	-	450
	FCC gasoline mode			616.3	1500	-
	FCC gas oil mode			-	-	-
	Hydrocracker			-	1105	2436.54
	Delayed coker			-	-	2066
	Des Gas oil			1390	2822.6	2383.8
	Des cycle gas oil			200	669	-
	Des ATK			-	762	1680
	Des Distillates			-	-	498
Intermediate streams exchange	**From**	**R1**	VGO	-	-	337.7
			VRSD	-	-	350
		R2	VRSD	-	-	319.5
		R3	HN	-	283.6	-
			CoGO	-	350	-
Exports	PG95				334.1	
	JP4				1433.6	
	GO6				3862	
	HFO				1203	
	ATK				1251.7	
	Coke				402.4	
	Diesel				230.6	
Total cost ($/yr)					6,885,000	

Scenario-3: multiple feedstocks, multiple refineries with integration. In this scenario, we provide multiple feedstocks, namely; Arabian Light and Kuwait crude, to the refineries complex and demonstrate the selection of crude combinations to each refinery as well as how the integration network will change. All sets of constraints remained the same except for the crude supply as we imposed a higher availability limit of 20,000 tones/year of each crude type. The results of the model are shown in Table 3.6.

Table 3.6 Model results of multisite refinery planning; Scenario-3

Process variables				**Results (1000 ton/yr)**		
				R1	**R2**	**R3**
Crude oil supply	Crude 1			3536	11835	4629
	Crude 2			964	-	5271
	Total			4500	11835	9900
Production levels	Crude unit			4500	11835	9900
	Reformer 95			227	-	-
	Reformer 100			736	1804	1074
	Isomerization			144	-	450
	FCC gasoline mode			485	1395	-
	FCC gas oil mode			-	-	-
	Hydrocracker			-	1741	2431
	Delayed coker			-	-	2066
	Des Gas oil			1121	2727	2127
	Des cycle gas oil			200	622	-
	Des ATK			-	1200	1676
	Des Distillates			-	-	498
Intermediate streams exchange	**From**	**R1**	VGO	-	265	-
			VRSD	-	-	24
		R3	HN	226	-	-
Exports	JP4				837	
	GO6				2860	
	HFO				2390	
	ATK				1794	
	Coke				402.4	
	Diesel				230.6	
Total cost ($/yr)					7,263,000	

The total crude oil supply to the refineries complex remained the same. However; the overall utilization of some major production units has changed. The capacity utilization of thermal and catalytic reactors has increased whereas reforming utilization has slightly decreased. This is because Kuwait crude contains more heavy ends as apposed to Arabian light which has more of the lighter ends. The selection of crude supply type was in favor of Arabian Light as it was processed up to its maximum availability level of 20,000 tones/year where the remaining required crude was fulfilled by Kuwait crude. Due to the shortage in Arabian Light supply, the model used Kuwait crude to satisfy local market demand although it yields a higher overall annual production cost of $ 7,263,000. This scenario illustrates the use of different combinations of crude types and how this affects the overall production units utilization, refineries network integration, and total annual cost. In the next scenario we will see how expanding some processes will increase other production units capacity utilization.

Scenario-4: multiple feedstocks, multiple refineries with integration and increased market demand. In all previous scenarios, we did not change the market demand and therefore there was no expansion in the production unit capacities of the refineries. In this scenario, we will simulate a change in market demand and examine the modifications suggested by the model. Table 3.7 illustrates the new major operating constraints.

In general, developing cost models of production system expansions only as a function of the unit flowrate does not provide a good capital cost estimate. For this reason and as we mentioned earlier, our formulation only allowed the addition of predetermined capacities whose price can be acquired a priori through design companies' quotations.

Table 3.7 Major refineries capacity constraints for multisite refinery planning, Scenario-4

	Higher limit (1000 ton/yr)		
Production Capacity	R1	R2	R3
Distillation	5000	12000	11000
Reforming	1000	2000	1800
Isomerization	200	-	450
Fluid catalytic cracker	1700	1700	-
Hydrocracker	-	2000	2500
Delayed coker	-	-	2200
Des gas oil	1900	3000	2400
Des cycle gas oil	200	750	-
Des ATK	-	1200	1680
Des Distillates	-	-	700
Crude availability			
Crude 1		20,000	
Crude 2		20,000	
Local Demand			
LPG		432	
LN		312	
PG98		540	
PG95		4440	
JP4		2340	
GO6		4920	
ATK		1800	
HFO		200	
Diesel		1200	
Coke		300	

Table 3.8 shows the new strategic plan for all refineries in terms of crude oil supply combinations, production expansions, and integration network design between the refineries. In response to the increase in the diesel production requirements by more than a double, the new plan suggests the installation of a new thermal coker and a distillates desulfurizatoin unit in Refinery 3. This change has a clear effect on the integration network design among the refineries. As an illustration, the new plan suggests to increase the level of intermediate exchange of vacuum residues from Refineries 1 and 2 to Refinery 3 in order to efficiently utilize the additional capacities of the coker and distillates desulfurizatoin units. The total

annual cost has increased to $ 21,463,000 due to the additional units' capital and operating costs.

Table 3.8 Model results of multisite refinery planning; Scenario-4

Process variables				Results (1000 ton/yr)		
				R1	**R2**	**R3**
Crude oil supply	Crude 1			3077	8293	6059
	Crude 2			1923	1333	4420
	Total			5000	9626	10479
Production levels	Crude unit			5000	9626	10479
	Reformer 95			276	-	19
	Reformer 100			724	2000	610
	Isomerization			163	-	450
	FCC gasoline mode			751	1595	-
	FCC gas oil mode			-	-	-
	Hydrocracker			-	1065	2500
	Delayed coker			-	-	3490
	Des Gas oil			1900	3000	1089
	Des cycle gas oil			200	712	-
	Des ATK			-	1200	1258
	Des Distillates			-	-	841
Intermediate streams exchange	**From**	**R1**	GO	-	52	-
			VGO	-	216	-
			VRSD	-	-	400
		R2	VRSD	-	-	400
		R3	HN	242	332	-
			GO	400	400	-
			ATK	-	240	-
			UCO	-	23	-
Process Expansions	Delayed Coker			-	-	1380
	Des Distillates			-	-	600
Exports	JP4				543	
	GO6				2655	
	HFO				1217	
	ATK				1272	
	Coke				886	
	Diesel				-	
Total cost ($/yr)					21,463,000	

3.6 Conclusion

A mixed-integer programming model for minimizing cost in the strategic planning of multirefineries network was presented. The objective was to develop a methodology for designing a process integration network and production capacity expansions in a multiple refinery complex using different feedstock alternatives. Two examples with multiple scenarios of large-scale refineries were solved to illustrate the performance of the proposed design methodology and to show the economic potential and trade-offs involved in the optimization of such systems. The integration specifically addressed intermediate material transfer between processing units at each site. In the formulation, bilinear mixing equations were avoided by introducing individual component flows in order to maintain linearity.

Petroleum refining is a central and crucial link in the oil supply chain and has received extensive attention over the last decades. However, despite all the progress that has been made in developing planning and scheduling models a general purpose model is still a target (Grossmann, 2005). A general model that can be used for different planning levels, short, medium and long range will be of great benefit in terms of seamless interactions of these functions. In this work we showed the capability of the proposed model in capturing all details required for medium-range and tactical planning as illustrated by Example 1. This is a step forward in achieving such vertical integration among all planning hierarchies.

In our study, all parameters were assumed to be deterministic. However, the current situation of fluctuating petroleum crude oil prices and demands is an indication that markets and industries everywhere are impacted by uncertainties. For example, source and availability of crude oils as the raw material; prices of feedstock, chemicals, and

commodities; production costs; and future market demand for finished products will have a direct impact on final decisions. Thus, acknowledging the shortcomings of deterministic models, the next phase of our investigation will be considering uncertainties in the design problem.

Chapter 4

Robust Optimization of Multisite Refinery Network: Integration and Coordination

4.1 Introduction

Today the petroleum refining industry is facing a challenging task to remain competitive in a globalized market. High crude oil prices and growing stringent international protocols and regulations force petroleum companies to embrace every opportunity that increases their profit margin. A common solution is to seek integration alternatives not only within a single facility but also on an enterprise-wide scale. This will provide enhanced utilization of resources and improved coordination and therefore achieve a global optimal production strategy within the network. However, considering such highly strategic planning decisions, particularly in the current volatile market and the ever changing customer requirements, uncertainties play a paramount role in the final decision making.

The remainder of Chapter 4 is organized as follows. In the following section we will give a review of the related literature. Section 4.3 will discuss the proposed model formulation for petroleum refining multisite network planning under uncertainty and using robust optimization. Then we will briefly explain the sample average approximation (SAA) method in section 4.4. In section 4.5, we will present computational results and the performance of the proposed approach on industrial case studies consisting of a single

refinery and a network of petroleum refineries. The chapter ends with concluding remarks in section 4.6.

4.2 Literature Review

Different approaches have been devised to tackle optimization under uncertainty including stochastic optimization (two-stage, multistage) with recourse based on the seminal work of Dantzig (1955), chance-constrained optimization (Charnes & Cooper, 1959), fuzzy programming (Bellman & Zadeh, 1970), and design flexibility (Grossmann and Sargent, 1978). These early works on optimization under uncertainty have undergone substantial developments in both theory and algorithms (Sahinidis, 2004). In this thesis, we employ stochastic programming with recourse which deals with problems with uncertain parameters of a given discrete or continuous probability distribution. The most common formulation of stochastic programming models for planning problems is the two-stage stochastic program. In a two-stage stochastic programming model, decision variables are cast into two groups: first stage and second stage variables. The first stage variables are decided prior to the actual realization of the random parameters. Once the uncertain events have unfolded, further design or operational adjustments can be made through values of the second-stage (alternatively called recourse variables at a particular cost). Stochastic programming with recourse commonly gives rise to large-scale models that require the use of decomposition methods and proper approximation techniques due to the high number of samples encountered (Liu & Sahinidis, 1996). However, recent developments in sampling techniques may help maintain the stochastic program to a manageable size.

More recent applications and developments in the chemical engineering arena include the work by Ierapetritou and Pistikopoulos (1994) who proposed an algorithm for a two-stage stochastic linear planning model. The algorithm is based on design flexibility by finding a feasible subspace of the probability region instead of enumerating all possible uncertainty realizations. They also developed a Benders decomposition scheme for solving the problem without a priori discretization of the random space parameters. This was achieved by means of Gaussian quadrature numerical integration of the continuous density function. In a similar production planning problem, Clay and Grossmann (1996) developed a successive disaggregation algorithm for the solution of two-stage stochastic linear models with discrete uncertainty. Liu and Sahinidis (1995; 1996; 1997) studied the design uncertainty in process expansion using sensitivity analysis, stochastic programming and fuzzy programming, respectively. In their stochastic model, they used Monte Carlo sampling to calculate the expected objective function values. Their comparison over the different methodologies was in favor of stochastic models when random the parameter distributions are not available. Ahmed et al. (2000) proposed a modification to the decomposition algorithm of Ierapetritou and Pistikopoulos (1994). They were able to avoid solving the feasibility subproblems and instead of imposing constraints on the random space, they developed feasibility cuts on the master problem of their decomposition algorithm. The modification mitigates suboptimal solutions and develops a more accurate comparison to cost and flexibility. Nerio and Pinto (2005) developed a multiperiod MINLP model for production planning of refinery operations under uncertain petroleum and product prices and demand. They were able to solve the model for 19 periods and five scenarios.

Another stream of research considered risk and robust optimization. The representation of risk management using variance as a risk measure was proposed by Mulvey et al. (1995) in which they referred to this approach as robust stochastic programming. They defined two types of robustness: a) solution robustness referring to the optimal model solution when it remains close to optimal for any scenario realization, and b) model robustness representing an optimal solution when it is almost feasible for any scenario realization. Ahmed and Sahinidis (1998) proposed the use of an upper partial mean (UPM) as an alternative measure of variability with the aim of eliminating nonlinearities introduced by using variance. In addition to avoiding nonlinearity of the problem, UPM presents an asymmetric measure of risk, as apposed to variance, by penalizing unfavorable risk cases. Bok et al. (1998) proposed a multiperiod robust optimization model for chemical process networks with demand uncertainty and applied it to the petrochemical industry in South Korea. They adopted the robust optimization framework by Mulvey et al. (1995) where they defined solution robustness as the model solution when it remains close to optimal for any demand realization, and model robustness when it has almost no excess capacity and unmet demand. More recently, Barbaro and Bagajewicz (2004) proposed a new risk metric to manage financial risk. They defined risk as the probability of not meeting a certain target profit, in the case of maximization, or cost, in the case of minimization. Additional binary variables are then defined for each scenario where each variable assumes a value of 1 in the case of not meeting the required target level; either profit or cost, and zero otherwise. Accordingly, appropriate penalty levels are assigned in the objective function. This approach mitigates the shortcomings of the symmetric penalization in the case of using variance, but on the other hand, adds computational burden through additional binary variables. Lin et al. (2004)

proposed a robust optimization approach based on min-max framework where they consider bounded uncertainty without known probability distribution. The uncertainty considered was both in the objective function coefficients and right-hand-side of the inequality constraints and was then applied to a set of MILP problems. This approach allowed the violation of stochastic inequality constraints with a certain probability and uncertainty parameters were estimated from their nominal values through random perturbations. This approach, however, could result in large infeasibilities in some of the constraints when the nominal data values are slightly changed. This work was then extended by Janak et al. (2007) to cover known probability distributions and mitigate the big violations of constraints in Lin et al. (2004) via bounding the infeasibility of constraints and finding "better" nominal values of the uncertain parameters. It is worth mentioning that both Lin et al. (2004) and Janak et al. (2007) work is based on infeasibility/optimality analysis and does not consider recourse actions. For recent reviews on scheduling problems under uncertainty, we refer the interested reader to Janak, et al. (2007) and for reviews on single and multisite planning and coordination see Chapter 3.

In this chapter, we extend the deterministic modeling for the design and analysis of multisite integration and coordination within a network of petroleum refineries proposed in Chapter 3 to consider uncertainty in raw materials and final product prices as well as products demand. This work also accounts for both model robustness and solution robustness, following the Mulvey et al. (1995) approach. The stochastic model is formulated as a two-stage stochastic MILP problem whereas the robust optimization is formulated as an MINLP problem with nonlinearity arising from modeling the risk components. The proposed approach tackles parameters uncertainty in the coefficients of the objective function and the right-hand-side of inequality constraints. Furthermore, we apply the sample average

approximation (SAA) method within an iterative scheme to generate the required samples. The solution quality is then statistically assessed by measuring the optimality gap of the final solution. The proposed approach was applied to industrial scale case studies of a single petroleum refinery and a network of refineries.

4.3 Model Formulation

4.3.1 Stochastic Model

The formulation addresses the problem of determining an optimal integration strategy across multiple refineries and establishing an overall production and operating plan for each individual site. The deterministic model was explained in Chapter 3. In this study, uncertainty is accounted for using two-stage stochastic programming with recourse. Parameters uncertainties considered in this study include uncertainties in the imported crude oil price $CrCost_{cr}$, product price Pr_{cfr}^{Ref}, (uncertainties in the coefficients of the objective function) and the market demand $D_{Ref_{cfr}}$ (uncertainties in the right hand side of inequality constraints). Uncertainty is modeled through the use of mutually exclusive scenarios of the model parameters with a finite number N of outcomes. For each $\xi_k = (CrCost_{cr,k}, Pr_{cfr,k}^{Ref}, D_{Ref_{cfr,k}})$ where $k = 1,2,...,N$, there corresponds a probability p_k. The generation of the scenarios as well as model statistical bounding will be explained in a later section. The stochastic model is given by:

$$
\begin{aligned}
Min \quad & \sum_{cr\in CR}\sum_{i\in I}\sum_{k\in N} p_k\, CrCost_{cr,k}\, S^{Ref}_{cr,i} + \sum_{p\in P} OpCost_p \sum_{cr\in CR}\sum_{i\in I} z_{cr,p,i} \\
& + \sum_{cir\in CIR}\sum_{i\in I}\sum_{i'\in I} InCost_{i,i'}\, ypipe^{Ref}_{cir,i,i'} + \sum_{i\in I}\sum_{m\in M_{Ref}}\sum_{s\in S} InCost_{m,s}\, yexp^{Ref}_{m,i,s} \\
& - \sum_{cfr\in PEX}\sum_{i\in I}\sum_{k\in N} p_k\, Pr^{Ref}_{cfr,k}\, e^{Ref}_{cfr,i} + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref+}_{cfr}\, V^{Ref+}_{cfr,k} \\
& + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref-}_{cfr}\, V^{Ref-}_{cfr,k}
\end{aligned}
\qquad \text{where } i \neq i' \tag{4.1}
$$

Subject to

$$
z_{cr,p,i} = S^{Ref}_{cr,i} \qquad \forall\ cr\in CR,\ i\in I \quad \text{where } p\in P' = \{\text{Set of CDU processes} \,\forall\, \text{plant i}\} \tag{4.2}
$$

$$
\sum_{p\in P}\alpha_{cr,cir,i,p}\ z_{cr,p,i} + \sum_{i'\in I}\sum_{p\in P}\xi_{cr,cir,i',p,i}\ xi^{Ref}_{cr,cir,i',p,i} - \sum_{i'\in I}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'} - \sum_{cfr\in CFR} w_{cr,cir,cfr,i} - \sum_{rf\in FUEL} w_{cr,cir,rf,i} = 0 \qquad \forall\ cr\in CR,\ cir\in CIR,\ i'\,\&\, i\in I \text{ where } i\neq i' \tag{4.3}
$$

$$
\sum_{cr\in CR}\sum_{cir\in CB} w_{cr,cir,cfr,i} - \sum_{cr\in CR}\sum_{rf\in FUEL} w_{cr,cfr,rf,i} = x^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ i\in I \tag{4.4}
$$

$$
\sum_{cr\in CR}\sum_{cir\in CB} \frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} = xv^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ i\in I \tag{4.5}
$$

$$
\sum_{cir\in FUEL} cv_{rf,cir,i}\ w_{cr,cir,rf,i} + \sum_{cfr\in FUEL} w_{cr,cfr,rf,i} - \sum_{p\in P}\beta_{cr,rf,i,p}\ z_{cr,p,i} = 0 \qquad \forall\ cr\in CR,\ rf\in FUEL,\ i\in I \tag{4.6}
$$

$$
\sum_{cr\in CR}\sum_{cir\in CB}\left(att_{cr,cir,q\in Qv}\ \frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} + att_{cr,cir,q\in Qw}\left[w_{cr,cir,cfr,i} - \sum_{rf\in FUEL} w_{cr,cfr,rf,i} \right] \right) \geq q^{L}_{cfr,q\in Qv}\ xv^{Ref}_{cfr,i} + q^{L}_{cfr,q\in Qw}\ x^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ q=\{Qw,Qv\},\ i\in I \tag{4.7}
$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\left(att_{cr,cir,q\in Qv}\ \frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}}+att_{cr,cir,q\in Qw}\left[w_{cr,cir,cfr,i}-\sum_{rf\in FUEL}w_{cr,cfr,rf,i}\right]\right) \le q^{U}_{cfr,q\in Qv}\ xv^{Ref}_{cfr,i}+q^{U}_{cfr,q\in Qw}\ x^{Ref}_{cfr,i} \qquad \begin{array}{l}\forall\\ cfr\in CFR,\\ q=\{Qw,Qv\},\\ i\in I\end{array} \qquad (4.8)$$

$$MinC_{m,i}\le\sum_{p\in P}\gamma_{m,p}\sum_{cr\in CR}z_{cr,p,i}\le MaxC_{m,i}+\sum_{s\in S}AddC_{m,i,s}\ y_{exp}{}^{Ref}_{m,i,s} \qquad \begin{array}{l}\forall\\ m\in M_{Ref},i\in I\end{array} \qquad (4.9)$$

$$\sum_{cr\in CR}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'}\le F^{U}_{cir,i,i'}\ y_{pipe}{}^{Ref}_{cir,i,i'} \qquad \begin{array}{l}\forall\ cir\in CIR,\ i'\ \&\ i\in I\\ \text{where } i\ne i'\end{array} \qquad (4.10)$$

$$\sum_{i\in I}\left(x^{Ref}_{cfr,i}-e^{Ref}_{cfr',i}\right)+V^{Ref+}_{cfr,k}-V^{Ref-}_{cfr,k}=D_{Ref_{cfr,k}} \qquad \begin{array}{l}cfr\in CFR\\ \forall\ cfr'\in PEX\\ k\in N\end{array} \qquad (4.11)$$

$$IM^{L}_{cr}\le\sum_{i\in I}S^{Ref}_{cr,i}\le IM^{U}_{cr} \qquad \forall\ cr\in CR \qquad (4.12)$$

The above formulation is a two-stage stochastic mixed-integer linear programming (MILP) model. Objective function (4.1) minimizes the first stage variables and the penalized second stage variables. Similar to the analysis of inventory problems (Ahmed et al., 2007), the production over the target demand is penalized as an additional inventory cost of each ton of refined products. Similarly, shortfall in a certain product demand is assumed to be satisfied at the product spot market price. The recourse variables $V^{Ref+}_{cfr,k}$ and $V^{Ref-}_{cfr,k}$ in equation (4.11) represent the shortfall and surplus for each random realization $k\in N$, respectively. These will compensate for the violations in equation (4.11) and will be

penalized in the objective function using appropriate shortfall and surplus costs C_{cfr}^{Ref+} and C_{cfr}^{Ref-}, respectively. Uncertain parameters are assumed to follow a normal distribution for each outcome of the random realization ξ_k. Although this might sound restrictive, this assumption bears no limitation to the generality of the proposed approach as other distributions can be easily used instead. The recourse variables $V_{cfr,k}^{Ref+}$ and $V_{cfr,k}^{Ref-}$ in this formulation will compensate for deviations from the mean of the market demand.

4.3.2 Robust Model

The above stochastic model takes a decision merely based on first-stage and expected second-stage costs leading to an assumption that the decision-maker is risk-neutral. The generic representation of risk can be written as:

$$Min_{x,y} \; c^T x + \mathrm{E}[Q(x,\xi(\omega))] + \lambda f(\omega, y)$$

where f is a measure of variability of the second-stage costs and λ is a non-negative scalar representing risk tolerance which is usually decided by the modeler. This representation is referred to as mean-risk model (Ahmed et al., 2007). This formulation follows the representation of the Markowitz mean–variance (MV) model (Markowitz, 1952). The variability measure can be modeled as variance, mean-absolute deviation or financial measures of Value-at-Risk (VaR) and Conditional Value-at-Risk (CVaR).

In this study, risk is modeled in terms of variance in both prices of imported crude oil $CrCost_{cr}$ and petroleum products Pr_{cfr}^{Ref}, represented by first stage variables, and forecasted demand $D_{Ref_{cfr}}$, represented by the recourse variables. The variability in the prices represents

the solution robustness in which the model solution will remain close to optimal for all scenarios. On the other hand, variability of the recourse term represents the model robustness in which the model solution will almost be feasible for all scenarios. This technique gives rise to a multiobjective optimization problem in which scaling factors are used to evaluate the sensitivity due to variations of each term. The variations in the raw material and product prices are scaled by θ_1 and the deviation from forecasted demand is scaled by θ_2. Different values of θ_1 and θ_2 are used in order to observe the sensitivity of each term on the final solution of the problem. The objective function with risk consideration can be written as shown in (4.13) below:

$$\begin{aligned} Min \quad & \sum_{cr\in CR}\sum_{i\in I}\sum_{k\in N} p_k\, CrCost_{cr,k}\, S^{Ref}_{cr,i} + \sum_{p\in P} OpCost_p \sum_{cr\in CR}\sum_{i\in I} z_{cr,p,i} \\ & + \sum_{cir\in CIR}\sum_{i\in I}\sum_{i'\in I} InCost_{i,i'}\; ypipe^{Ref}_{cir,i,i'} + \sum_{i\in I}\sum_{m\in M_{Ref}}\sum_{s\in S} InCost_{m,s}\; yexp^{Ref}_{m,i,s} \\ & - \sum_{cfr\in PEX}\sum_{i\in I}\sum_{k\in N} p_k\, Pr^{Ref}_{cfr,k}\, e^{Ref}_{cfr,i} + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref+}_{cfr}\, V^{Ref+}_{cfr,k} \\ & + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref-}_{cfr}\, V^{Ref-}_{cfr,k} + \theta_1\left[\sqrt{\mathrm{var}(CrCost_{cr,k}\, S^{Ref}_{cr,i})} + \sqrt{\mathrm{var}(Pr^{Ref}_{cfr,k}\, e^{Ref}_{cfr,i})}\right] \\ & + \theta_2\left[\sqrt{\mathrm{var}(C^{Ref+}_{cfr}\, V^{Ref+}_{cfr,k})} + \sqrt{\mathrm{var}(C^{Ref-}_{cfr}\, V^{Ref-}_{cfr,k})}\right] \end{aligned} \tag{4.13}$$

By expanding the mean and variance terms of $CrCost_{cr,k}$, $Pr^{Ref}_{cfr,k}$, $V^{Ref+}_{cfr,k}$ and $V^{Ref-}_{cfr,k}$, the objective function (4.13) can be recast as:

$$
\begin{aligned}
Min \quad & \sum_{cr\in CR}\sum_{i\in I}\sum_{k\in N} p_k\, CrCost_{cr,k}\, S^{Ref}_{cr,i} + \sum_{p\in P} OpCost_p \sum_{cr\in CR}\sum_{i\in I} z_{cr,p,i} \\
& + \sum_{cir\in CIR}\sum_{i\in I}\sum_{i'\in I} InCost_{i,i'}\, ypipe^{Ref}_{cir,i,i'} + \sum_{i\in I}\sum_{m\in M_{Ref}}\sum_{s\in S} InCost_{m,s}\, yexp^{Ref}_{m,i,s} \\
& - \sum_{cfr\in PEX}\sum_{i\in I}\sum_{k\in N} p_k\, Pr^{Ref}_{cfr,k}\, e^{Ref}_{cfr,i} + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref+}_{cfr}\, V^{Ref+}_{cfr,k} \\
& + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref-}_{cfr}\, V^{Ref-}_{cfr,k} \\
& + \theta_1 \left(\sqrt{\sum_{cr\in CR}\sum_{i\in I}\sum_{k\in N} (S^{Ref}_{cr,i})^2\; p_k \left[CrCost_{cr,k} - \sum_{k\in N} p_k\, CrCost_{cr,k} \right]^2} \right. \\
& \left. + \sqrt{\sum_{cr\in CR}\sum_{i\in I}\sum_{k\in N} (e^{Ref}_{cfr,i})^2\; p_k \left[Pr^{Ref}_{cfr,k} - \sum_{k\in N} p_k\; Pr^{Ref}_{cfr,k} \right]^2} \right) \\
& + \theta_2 \left(\sqrt{\sum_{cfr\in CFR}\sum_{k\in N} \left[C^{Ref+}_{cfr}\right]^2 p_k \left[V^{Ref+}_{cfr,k} - \sum_{k\in N} p_k\, V^{Ref+}_{cfr,k} \right]^2} \right. \\
& \left. + \sqrt{\sum_{cfr\in CFR}\sum_{k\in N} \left[C^{Ref-}_{cfr}\right]^2 p_k \left[V^{Ref-}_{cfr,k} - \sum_{k\in N} p_k\, V^{Ref-}_{cfr,k} \right]^2} \right)
\end{aligned}
\tag{4.14}
$$

In order to understand the effect of each term on the overall objective function of the system, different values of θ_1 and θ_2 are evaluated to construct the efficient frontier of expected cost versus risk measured by standard deviation. This will be demonstrated in the illustrative case studies.

4.4 Sample Average Approximation (SAA)

4.4.1 SAA Method

The solution of stochastic problems is generally very challenging as it involves numerical integration over the random continuous probability space of the second stage variables (Goyal & Ierapetritou, 2007). An alternative approach is the discretization of the random space using a finite number of scenarios. This approach has received increasing attention in the literature since it gives rise to a deterministic equivalent formulation which can then be

solved using available optimization algorithms. A common approach is Monte Carlo sampling where independent pseudo-random samples are generated and assigned equal probabilities (Ruszczyński and Shapiro, 2003).

The use of numerical integration through Gaussian Quadratures and Cubatures was studied by Pistikopoulos and Ierapetritou (1995). Acevedo and Pistikopoulos (1996) compared the Gaussian numerical integration methods with Monte Carlo sampling technique and suggested the use of Cubature methods for smaller dimensional problems and sampling-based methods for larger problems. The sampling-based methods were further classified by Verweij et al. (2003) to either "interior" or "exterior" sampling. In the interior sampling approach, samples can be adjusted during the optimization procedure by either adding additional samples to the previously generated ones, taking subsets of the samples, or even by generating completely new samples. Examples of this approach include the stochastic decomposition algorithm by Higle and Sen (1991) and the branch and bound algorithm by Norkin et al. (1998). On the other hand, exterior sampling includes the class of problems where samples are generated "outside" the optimization algorithm and then use the samples to construct and solve the problem as a deterministic equivalent. The Sample Average Approximation (SAA) method, also known as stochastic counterpart, is an example of an exterior sampling approach. The Sample Average Approximation problem can be written as (Verweij et al., 2003):

$$\nu_N = \min_{x \in X} c^T x + \frac{1}{N} \sum_{k \in N} Q(x, \xi^k) \tag{4.15}$$

It approximates the expectation of the stochastic formulation (usually called the "true" problem) and can be solved using deterministic algorithms. The SAA method was used

among others by Shapiro and Homemde-Mello (1998), Mark et al. (1999), Linderoth et al. (2002) for stochastic linear problems, Kleywegt et al. (2001), Verweij et al. (2003) for stochastic integer problems, and Wei and Realff (2004), Goyal and Ierapetritou (2007) for MINLP problems. Problem (4.15) can be solved iteratively in order to provide statistical bounds on the optimality gap of the objective function value. For details and proofs see Norkin et al. (1998) and Mark et al. (1999). The procedure consists of a number of steps as described in the following section.

4.4.2 SAA Procedure

- Generate R independent sample batches (denoting the number of sample replication) each with sample size of N, i.e. $\xi^{j1},...,\xi^{jN}$, $j=1,...,R$. For each sample size N solve the sample average approximation problem defined as:

$$v_N^j = \min_{x\in X} c^T x + \frac{1}{N}\sum_{k\in N} Q(x,\xi^{kj}) \tag{4.16}$$

  The objective values $v_N^1,...v_N^R$ of problem (4.16) and their corresponding solutions $\hat{x}_N^1,...\hat{x}_N^R$ are then obtained.

- Calculate:

$$\overline{v}_N = \frac{1}{R}\sum_{j\in R} v_N^j \tag{4.17}$$

$$\frac{\sigma^2_{\overline{v}_N}}{R} = \frac{1}{R(R-1)}\sum_{j\in R}(v_N^j - \overline{v}_N)^2 \tag{4.18}$$

According to Mark et al. (1999) and Norkin et al. (1998), the value of $\overline{v}_N$ in (4.17) is less than or equal to the true optimal value v^* obtained by solving the "true" problem, see Appendix for proof. Therefore, $\overline{v}_N$ is a statistical lower bound to the true optimal value with a variance estimator of $\frac{\sigma^2_{\overline{v}_N}}{R}$ calculated by equation (4.18).

- Select any candidate solution $\hat{x}^1_N,...\hat{x}^R_N$ obtained from the previous steps. However, it is preferable to select the optimal solution with the minimum objective function value, that is:

$$\hat{x}^* \in \arg\min\,[v^R_N : \hat{x}^1_N, \hat{x}^2_N, \ldots, \hat{x}^R_N] \tag{4.19}$$

- Fix the solution value to the point obtained from the above minimization in (4.19); generate an independent sample $N' = \xi^1,...,\xi^{N'}$ and compute the value of the following objective function:

$$\hat{v}_{N'} = \min_{\hat{x}^*} c^T\hat{x}^* + \frac{1}{N'}\sum_{k\in N'} Q(\hat{x}^*, \xi^k) \tag{4.20}$$

Considering the relatively less computational effort required to solve problem (4.20), the value of N' is typically chosen to be quite larger than N in order to obtain an accurate estimation of $\hat{v}_{N'}$ (Verweij et al., 2003). Since $\hat{x}^*$ is a feasible point to the true problem, we have $\hat{v}_{N'} \geq v^*$. Hence, $\hat{v}_{N'}$ is a statistical upper bound to the true problem with a variance estimated by equation (4.21):

$$\frac{\sigma^2_{\hat{v}_{N'}}}{N'} = \frac{1}{N'(N'-1)}\sum_{k\in N'}(c^T\hat{x}^* + Q(\hat{x}^*, \xi^k) - \hat{v}_{N'})^2 \tag{4.21}$$

- From the above procedure, we can estimate the $(1-\alpha)$ confidence interval of the optimal gap. For a given $t_{n-1,\alpha/2}$ where t is critical value of the t-distribution with $(n-1)$ degrees of freedom, the following can be estimated:

$$\widetilde{\varepsilon}_l = t_{n-1,\alpha/2}\frac{\sigma_{\bar{v}_N}}{\sqrt{R}} \quad \text{and} \quad \widetilde{\varepsilon}_u = t_{n-1,\alpha/2}\frac{\sigma_{\hat{v}_{N'}}}{\sqrt{N'}}$$

- Then, the optimality gap can be constructed as:

$$[0, \{\hat{v}_{N'} - \bar{v}_N\}^+ + \widetilde{\varepsilon}_u + \widetilde{\varepsilon}_l \] \qquad \text{where } \{y\}^+ \equiv \max(y, 0). \tag{4.22}$$

Note that due to sampling error we may find that $\hat{v}_{N'} < \bar{v}_N$. For this reason the confidence interval obtained by (4.22) provides a more conservative bounding. The above procedure for the validation of a candidate solution was originally suggested by Norkin et al. (1998) and further developed by Mark et al. (1999).

4.5 Illustrative Case Study

This section presents computational results of the models and the sampling scheme proposed in this chapter. The refinery examples considered represent industrial-scale size refineries and an actual configuration that can be found in may industrial sites around the world. In the presentation of the results, we focus on demonstrating the sample average approximation computational results as we vary the sample sizes and compare their solution accuracy and the CPU time required for solving the models.

The modeling system GAMS (Brooke et al., 1996) is used for setting up the optimization models. The computational tests were carried out on a Pentium M processor 2.13 GHz. The models were solved with DICOPT (Viswanathan & Grossmann, 1990). The NLP

subproblems were solved with CONOPT2 (Drud, 1994), while the MILP master problems were solved with CPLEX (CPLEX Optimization Inc, 1993).

4.5.1 Single Refinery Planning

This example illustrates the performance of the proposed approach on a single site total refinery planning problem. The refinery scale, capacity and configuration mimic an existing refinery in the Middle East. Figure 4.1 is a state equipment network (SEN) representation of multiple refineries network, where in this example we will study Refinery 1. The refinery uses a single feedstock (Arabian Light) to feed the atmospheric crude unit where it separates crude oil into several fractions including LPG, naphtha, kerosene, gas oil and residues. The heavy residues are then sent to the vacuum unit where they are further separated into vacuum gas oil and vacuum residues. In general, depending on the production targets, different processing and treatment processes are applied to the crude fractions. In our case, the naphtha is further separated into heavy and light naphtha. Heavy naphtha is sent to the catalytic reformer unit to produce high octane reformates for gasoline blending and light naphtha is sent to light naphtha pool and to an isomerization unit to produce isomerate for gasoline blending too.

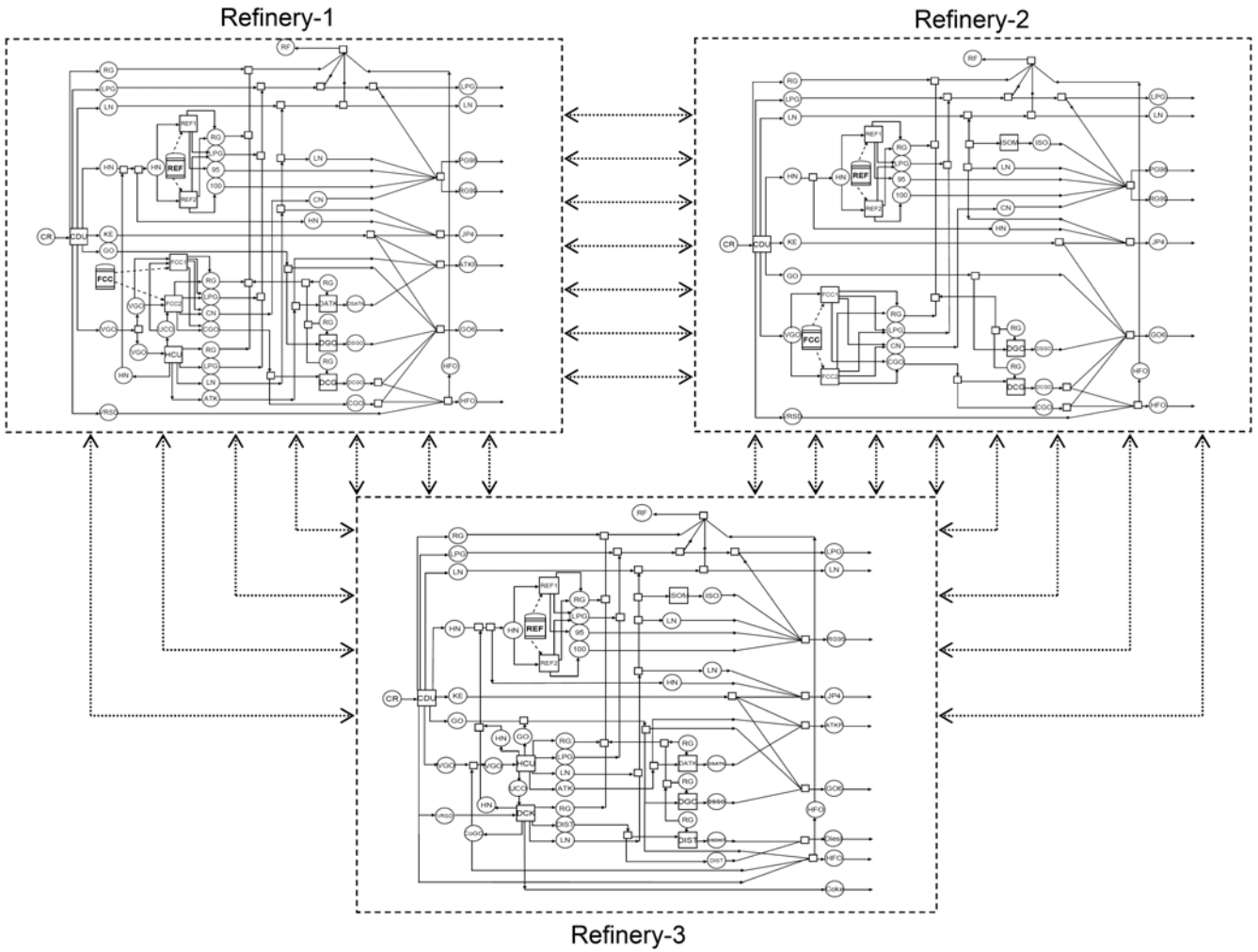

Figure 4.1 SEN representation of multiple refineries integration network.

The middle distillates are combined with other similar intermediate streams and sent for hydrotreating and then for blending to produce jet fuels and gas oils. Atmospheric and vacuum gas oils are further treated by either fluid catalytic cracking (FCC) or hydrocracking (HC) in order to increase the gasoline and distillate yields. These distillates from both FCC and HC are desulfurized in the cycle gas oil desulfurization and ATK desulfurization processes. The final products in this example consist of liquefied petroleum gas (LPG), light naphtha (LT), two grades of gasoline (PG98 and PG95), No.4 jet fuel (JP4), military jet fuel (ATKP), No.6 gas oil (GO6), and heating fuel oil (HFO).

The major capacity limitations as well as the availability constraints are shown in Table 4.1. Raw materials, product prices, and demand uncertainty were assumed to follow a normal distribution. However, this assumption bears no restriction to the generality of the proposed modeling approach as other sampling distributions can be easily used instead. Prices of crude oil and refined products reflect the current market prices and assume a standard deviation of $10 US. The problem is formulated as an LP since there is no integration or capacity expansion requirement in this case study.

Table 4.2 and Figure 4.2 show different confidence interval values of the optimality gap when changing the sample sizes of N and N', while fixing the number of replications R to 30. The replication number R need not be very large since usually 5 to 7 replications are sufficient to get an idea about the variability of $\overline{v}_N$ (Qian & Shapiro, 2006). It can be seen that the increase of the sample size N has more weight on reducing the optimality gap and therefore the variability of the objective function as compared to N'.

Table 4.1 Major capacity constraints of single refinery planning

	Higher limit (1000 ton/yr)
Production Capacity	
Distillation	12000
Reforming	2000
Fluid catalytic cracker	1000
Hydrocracker	2000
Des gas oil	3000
Des cycle gas oil	100
Des ATK	1200
Crude availability	
Arabian Light	12000
Local Demand	
LPG	$\mathcal{N}(320,20)$
LN	$\mathcal{N}(220,20)$
PG98	$\mathcal{N}(50,5)$
PG95	$\mathcal{N}(1600,20)$
JP4	$\mathcal{N}(1300,20)$
GO6	$\mathcal{N}(2500,50)$
ATKP	$\mathcal{N}(500,20)$
HFO	$\mathcal{N}(700,20)$

However, the increase of the sample size N will depend on computational time and available computer's memory. In our particular case studies, we run into memory limitations when we increase the sample size N beyond 2000 samples. Table 4.3 shows the solution of the single refinery problem using the SAA scheme with $N = 2000$ and $N' = 20000$. The proposed approach required 553 CPU sec to converge to the optimal solution.

The single refinery was then solved considering risk in terms of variations in the price of imported crude oil, prices of final products and forecasted demand to provide a more robust analysis of the problem. The problem was formulated as an NLP problem with nonlinearity due to modeling risk in terms of variance. As mentioned earlier, the problem will have a

more robust solution as the results will remain close to optimal for all scenarios through minimizing variations of the raw material and product prices. In a similar analogy, the

Table 4.2 Computational results with SAA of single refinery planning

		Lower bound sample size=N			
		500	1000	1500	2000
U B Sample Size	Number of Samples: R=30				
N'=5000	LB estimate: $\overline{v}_N$	2888136	2888660	2888964	2888978
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	1834	1446	1050	1036
	UB estimate: $\hat{v}_{N'}$	2889367	2889076	2889720	2887545
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	3636	3693	3653	3637
	95% Conf. Interval	[0,6701]	[0,5555]	[0,5458]	[0,4673]
	CPU (sec)	26	33	41	49
N'=10000	LB estimate: $\overline{v}_N$	2887536	2889941	2888123	2888526
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	2367	1311	1045	1332
	UB estimate: $\hat{v}_{N'}$	2887864	2890973	2888884	2888706
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	2574	2608	2601	2619
	95% Conf. Interval	[0,5269]	[0,4951]	[0,4407]	[0,4131]
	CPU (sec)	109	113	117	128
N'=20000	LB estimate: $\overline{v}_N$	2888639	2889023	2888369	2888293
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	2211	1604	1190	1090
	UB estimate: $\hat{v}_{N'}$	2889593	2889033	2888527	2888311
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	1841	1847	1835	1840
	95% Conf. Interval	[0,5006]	[0,3462]	[0,3183]	[0,2949]
	CPU (sec)	534	536	545	553

model will be more robust as we are minimizing the variations of the recourse variables (demand) leading to a solution that is almost feasible for all scenarios. The effect of each robustness term was evaluated by varying their scaling factors. The model was repeatedly solved for different values of θ_1 (price variations) and θ_2 (demand variations) in order to construct the efficient frontier plot of expected cost versus risk measured by standard deviation.

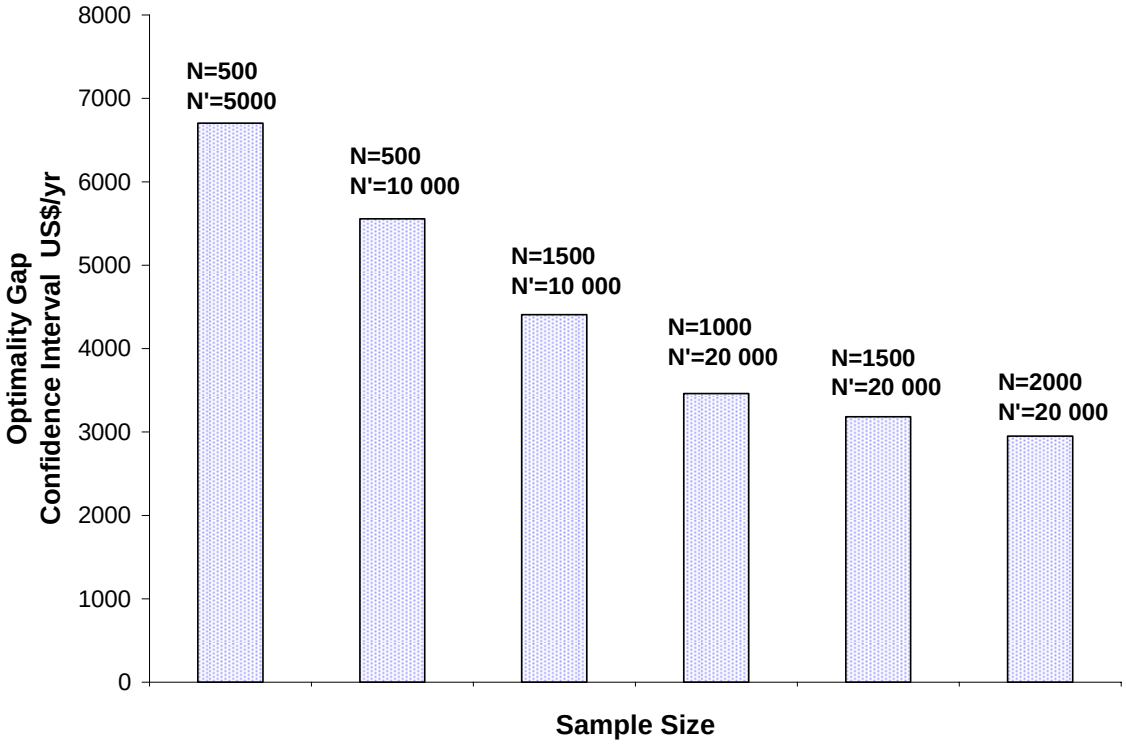

Figure 4.2 Single refinery planning optimality gap variations with sample size.

Table 4.3 Model results of single refinery planning

Process variables		Results (1000 ton/yr)
Production levels	Crude unit	12000
	Reformer 95	-
	Reformer 100	1824
	FCC gasoline mode	96
	FCC gas oil mode	708
	Hydrocracker	1740
	Des Gas oil	2891
	Des cycle gas oil	45
	Des ATK	1200
Exports	PG95	463
	JP4	502
	GO6	1293
	ATKP	1036
	HFO	1253
Total cost ($/yr)		2887687

Figure 4.3 illustrates the change in cost with respect to different values of θ_1 (price variations) and θ_2 (demand variations). The cost tends to increase as higher scaling values are given to the standard deviation of prices and demand. It can be seen from the graph that the problem bears more sensitivity to variations in raw material and product prices as compared to the variations in demand. Figure 4.4 illustrates the tradeoff between the expected cost vs. risk, represented by the total standard deviation of prices and demand. The expected cost decreases at higher values of risk in terms of price and demand variations with respect to different θ_1 and θ_2 values. Generally, the values of θ_1 and θ_2 will depend on the policy adopted by the investor or the plant operator whether they are risk-averse or risk takers and can be read directly from the efficient frontier plots.

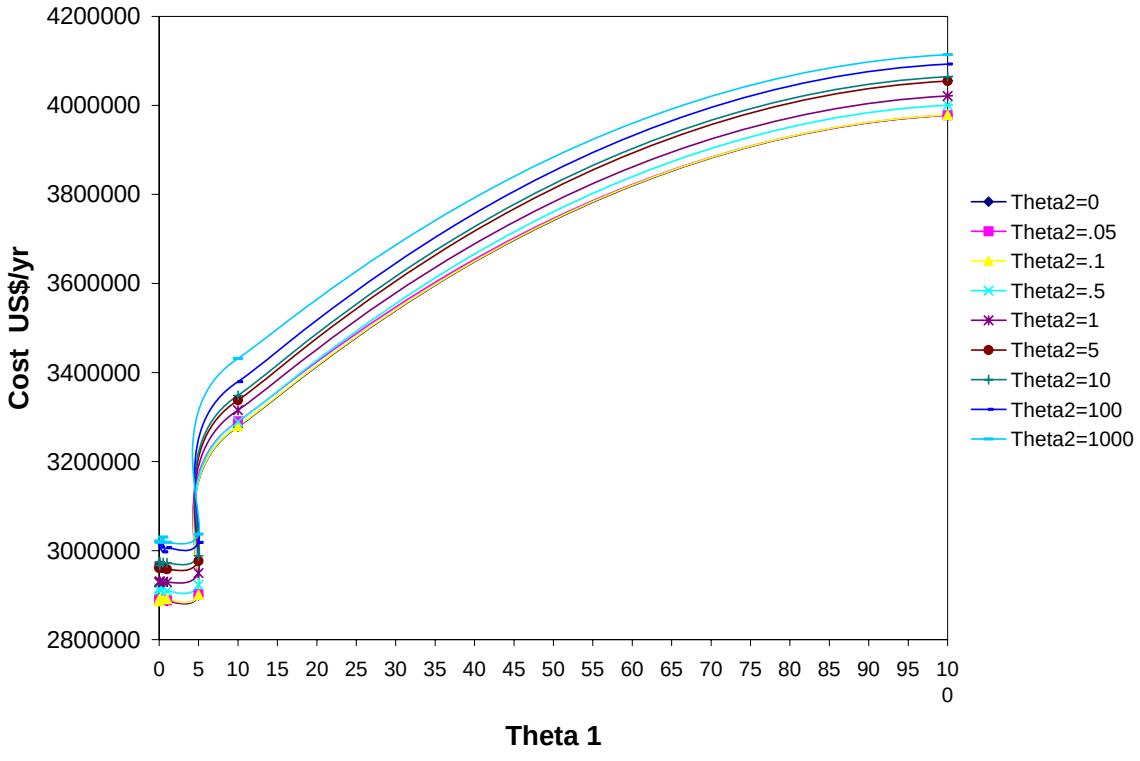

Figure 4.3 Cost variation with different values of θ_1 and θ_2 for single refinery planning.

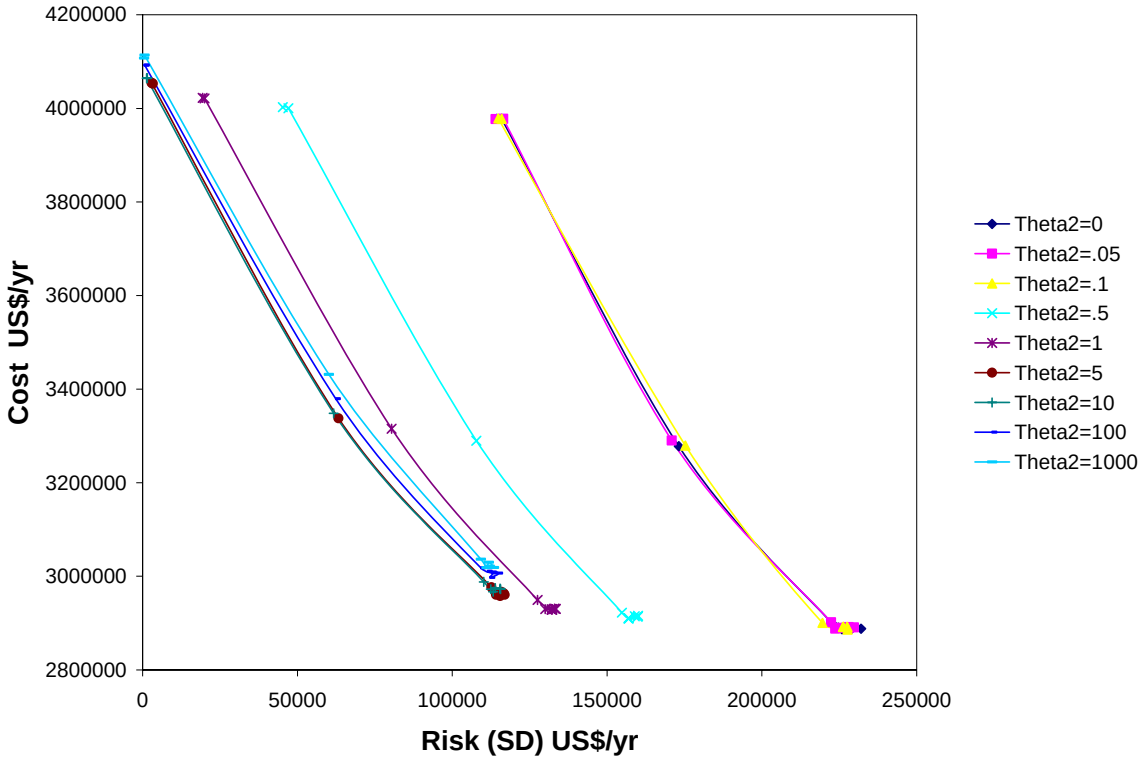

Figure 4.4 Tradeoff between cost and risk at different θ_2 values while varying θ_1 for single refinery planning.

4.5.2 Multisite Refinery Planning

In this example, we extend the scale of the case study to cover strategic planning for three complex refineries by which we demonstrate the performance of our model to devise an overall production plan and an integration strategy. See Figure 4.1 for the overall topology of the refineries and Table 4.4 for major capacity constraints. The three refineries are assumed to be in one industrial area, which is a common situation in many locations around the world, and are coordinated through a main headquarter sharing the feedstock supply. The cost parameters for pipeline installation were calculated as cost per distance between the refineries, and then multiplied by the required pipe length in order to connect any two refineries. The pipeline diameters considered in all cases was 8 inches. The final products of

the three refineries consist of liquefied petroleum gas (LPG), light naphtha (LT), two grades of gasoline (PG98 and PG95), No. 4 jet fuel (JP4), military jet fuel (ATKP), No.6 gas oil (GO6), diesel fuel (Diesel), heating fuel oil (HFO), and petroleum coke (coke). This problem was formulated as an MILP with the overall objective of minimizing total annualized cost.

Table 4.4 Major refineries capacity constraints for multisite refinery planning

	Higher limit (1000 ton/yr)		
Production Capacity	R1	R2	R3
Distillation	4500	12000	9900
Reforming	1000	2000	1800
Isomerization	200	-	450
Fluid catalytic cracker	800	1200	-
Hydrocracker	-	2000	2500
Delayed coker	-	-	1500
Des gas oil	1300	3000	2400
Des cycle gas oil	200	750	-
Des ATK	-	1200	1680
Des Distillates	-	-	350
Crude availability			
Arabian Light		31200	
Local Demand			
LPG		$\mathcal{N}$(432,20)	
LN		$\mathcal{N}$(250,20)	
PG98		$\mathcal{N}$(540,20)	
PG95		$\mathcal{N}$(4440,50)	
JP4		$\mathcal{N}$(2340,50	
GO6		$\mathcal{N}$(4920,50)	
ATK		$\mathcal{N}$(1800,50)	
HFO		$\mathcal{N}$(200,20)	
Diesel		$\mathcal{N}$(400,20)	
Coke		$\mathcal{N}$(300,20)	

Similar to the single refinery planning example in section 4.5.1, the problem was solved for different sample sizes N and N' to illustrate the variation of optimality gap confidence intervals as shown in Table 4.5 and Figure 4.5. The results illustrate the trade-off between model solution accuracy and computational effort. Furthermore, the increase of the sample

size N has a more pronounced effect on reducing the optimality gap, however, due to computational and memory limitations we did not increase the sample size N beyond 2000 samples.

Table 4.5 Computational results with SAA of the multisite refinery planning

		Lower bound sample size=N			
		500	1000	1500	2000
UB Sample Size	Number of Samples: R=30				
N'=5000	LB estimate: $\overline{v}_N$	6647411	6647713	6647569	6647109
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	4752	3185	2667	2516
	UB estimate: $\hat{v}_{N'}$	6661697	6658832	6656480	6652869
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	7877	7850	7746	7769
	95% Conf. Interval	[0,26915]	[0,22154]	[0,19325]	[0,16044]
	CPU (sec)	38	44	60	69
N'=10000	LB estimate: $\overline{v}_N$	6647660	6649240	6648294	6650178
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	3868	3750	2280	2105
	UB estimate: $\hat{v}_{N'}$	6656195	6658611	6656763	6655654
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	5447	5550	5463	5550
	95% Conf. Interval	[0,17850]	[0,18671]	[0,16213]	[0,13132]
	CPU (sec)	147	158	160	173
N'=20000	LB estimate: $\overline{v}_N$	6647296	6649123	6649634	6649421
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	3924	3248	2173	1720
	UB estimate: $\hat{v}_{N'}$	6656006	6656778	6656684	6654684
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	3923	3924	3895	3879
	95% Conf. Interval	[0,16557]	[0,14828]	[0,13118]	[0,10862]
	CPU (sec)	748	763	770	790

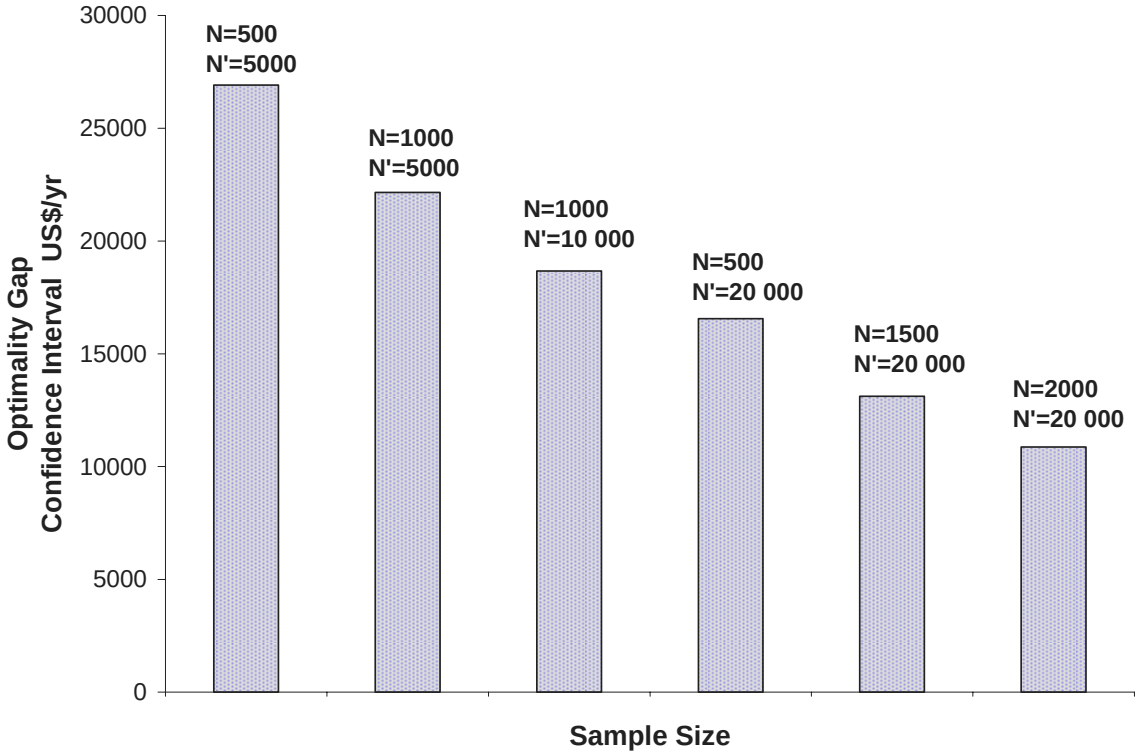

Figure 4.5 Multisite refinery planning optimality gap variations with sample size.

Table 4.6 shows the solution of the refineries network using the SAA scheme with N = 2000 and N' =20000 where the proposed model required 790 CPU sec to converge to the optimal solution. In addition to the master production plan devised for each refinery, the solution proposed the amounts of each intermediate stream to be exchanged between the different processes in the refineries. The formulation considered the uncertainty in the imported crude oil prices, petroleum product prices and demand. The three refineries collaborate to satisfy a given local market demand where the model provides the production and blending level targets for the individual sites. The annual production cost across the facilities was found to be $6,650,868.

Table 4.6 Model results of the multisite refinery planning

Process variables				Results (1000 ton/yr)		
				R1	**R2**	**R3**
Crude oil supply	Arabian Light			4500	12000	9900
Production levels	Crude unit			4500	12000	9900
	Reformer 95			172	539	-
	Reformer 100			401	1285	1772
	Isomerization			200	-	450
	FCC gasoline mode			616	1033	-
	FCC gas oil mode			-	-	-
	Hydrocracker			-	1740	2436
	Delayed coker			-	-	1100
	Des Gas oil			1035	2760	2378
	Des cycle gas oil			200	536	-
	Des ATK			-	1200	1680
	Des Distillates			-	-	264
Intermediate streams exchange	**From**	**R1**	VGO	-	-	338 to HCU
			CGO	-	75 to DCGO	-
		R2	LN	60 to Isom.	-	295 to Isom.
		R3	UCO	-	134 to FCC	-
Exports	PG95				296	
	JP4				1422	
	GO6				3657	
	HFO				1977	
	ATK				1837	
	Coke				40	
Total cost ($/yr)					6,650,868	

When considering risk, in an analogous manner to the single refinery case, the problem was solved for different values of θ_1 and θ_2 to construct the efficient frontier plot. Figure 4.6 illustrates how cost increases with respect to higher values of θ_1 and θ_2. The cost of operating the multisite refinery network will depend on the scaling values assigned to prices and demand variations. Figure 4.7 demonstrates the tradeoff between the cost and the total standard deviation of both prices and demand, denoted as risk. The figures show that the cost of production and designing the integration network between the refineries is more sensitive to variations in crude cost and product prices when compared to demand variations.

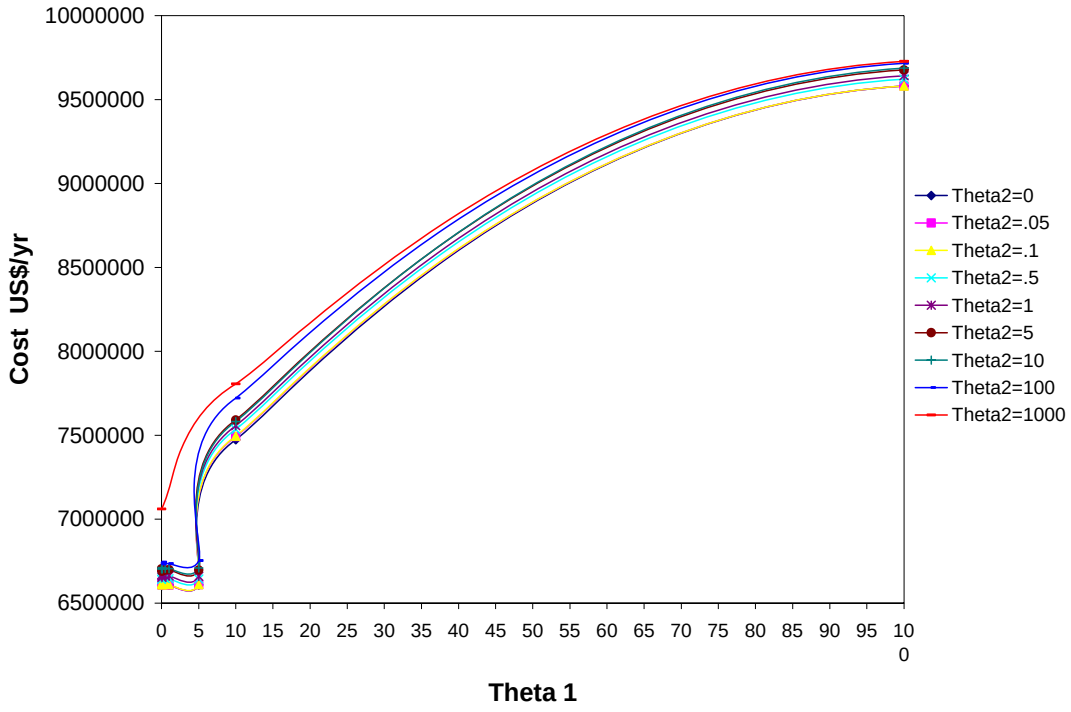

Figure 4.6 Cost variation with different values of θ_1 and θ_2 for multisite refinery planning.

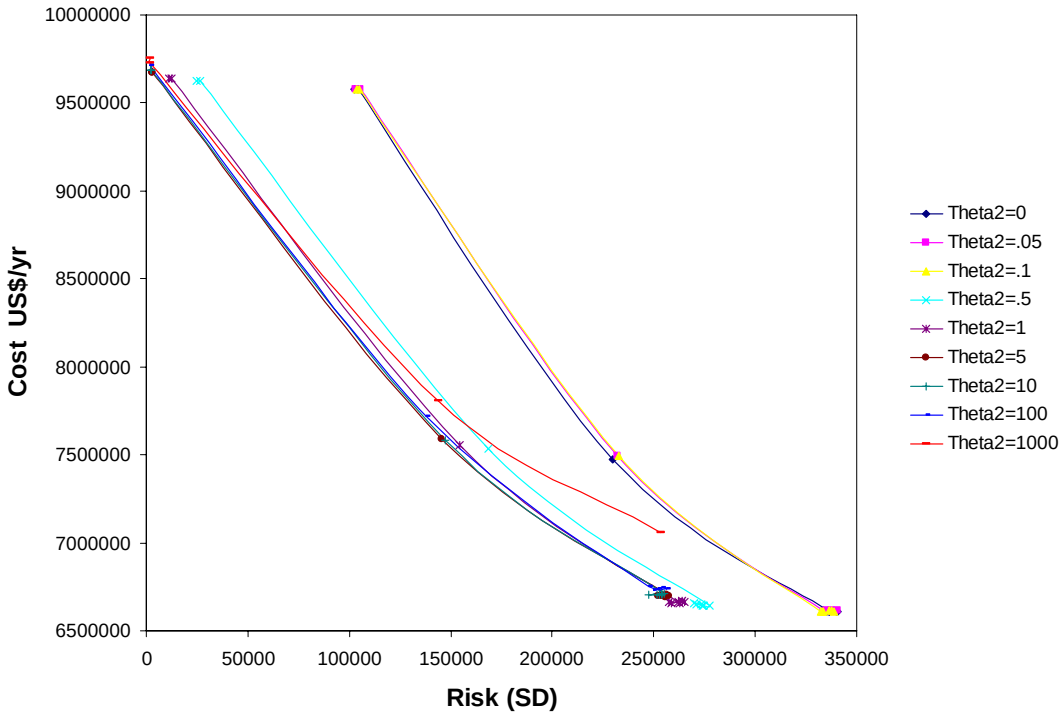

Figure 4.7 Tradeoff between cost and risk at different θ_2 values while varying θ_1 for multisite refinery planning.

Furthermore, for values of θ_1 and θ_2 exceeding 100, the model did not recommend exchange of intermediate streams between the refineries due to the high risk associated with such investment. However, the values of both θ_1 and θ_2 are left to the decision maker preference.

4.6 Conclusion

In this work, we proposed a two-stage stochastic MILP model for designing an integration strategy under uncertainty and plan capacity expansions, as required, in a multisite refinery network. The proposed method employs the sample average approximation (SAA) method with a statistical bounding and validation technique. In this sampling scheme, a relatively small sample size N is used to make decisions, with multiple replications, and another independent larger sample is used to reassess the objective function value while fixing the first stage variables and solving for the second stage variables. In addition, robust optimization of the refinery network integration model was also evaluated. The proposed approach led to results that are more stable against variability in imported crude oil and product prices (solution robustness) as well as forecasted product demand (model robustness). Furthermore, the study showed that the refinery models bear more sensitivity to variations in prices of imported crude oil and exported final products as apposed to variations in product demand. The scaling values of the solution and model robustness depend on the policy adopted by the investor whether being risk-averse or risk taker and can be read directly from the efficient frontier plots presented in this chapter.

Chapter 5

Optimization of Petrochemical Networks: Deterministic Approach

5.1 Introduction

The petrochemical industry is a network of highly integrated production processes where products of one plant may have an end use or may also represent raw materials for other processes. This flexibility in petrochemical products production and the availability of many process technologies offer the sense of switching between production methods and raw materials utilization. The world economic growth and increasing populations will keep global demand for transportation fuels and petrochemical products growing rapidly for the foreseeable future. One half of the petroleum consumption over the period of 2003 to 2030 will be in the transportation sector, whereas the industrial sector accounts for a 39-percent of the projected increase in world oil consumption, mostly for chemical and petrochemical processes (EIA, 2006). Meeting this demand will require large investments and proper strategic planning for the petrochemical industry.

The objective of this chapter is to give an overview on the optimization of petrochemical networks and set up the deterministic model which will be used in the analysis of parameter uncertainties in Chapter 6.

The remainder of Chapter 5 is organized as follows. In the following section we will review the related literature in the area of petrochemical planning. Then, we will discuss the deterministic model formulation for the petrochemical network planning and illustrate its performance through an industrial case study in section 5.3 and 5.4, respectively. The chapter ends with concluding remarks in section 5.5.

5.2 Literature Review

The realization of the petrochemical planning needs along with its important impact has inspired a great deal of research in order to devise different modeling frameworks and algorithms. These include optimization models with continuous and mixed-integer programming under both deterministic and uncertainty considerations.

The seminal work of Stadtherr and Rudd (1976, 1978) defined the petrochemical industry as a network of chemical process systems with linear chemical transformations and material interactions. They showed that the model provided a good representation of the petrochemical industry and can be used as a tool for estimating the relative effectiveness of available and new technologies and their impact on the overall industry. Their objective was to minimize feedstock consumptions. A similar LP modeling approach was adapted by Sokic and Stevancevic (1983). Sophos et al. (1980) presented a model that minimizes feedstock consumption and entropy creation (lost work). Fathi-Afshar and Yang (1985) devised a multiobjective model of minimizing cost and gross toxicity emissions. Modeling the petrochemical industry using linear programming may have showed its ability to provide relatively reliable results through different technology structures. However, the need for approximating non-linear objective functions or the restriction of process technology

combination alternatives mandated different modeling techniques involving mixed-integer programming.

Some of the first mixed-integer programming models that tackled this problem were proposed by Jimenez et al. (1982) and Jimenez and Rudd (1987) for the development of the Mexican petrochemical industry. The proposed models were used to plan the installation of new plants with profitable levels as opposed to importing chemical products. However, there were no capacity limitations constraints on the processes. Al-Amir et al. (1998) developed an MILP model for the development of Saudi Arabia's petrochemical industry maximizing profit. The model included minimum economic production quantity for the different processes and accounted for domestic consumption and global market exports. This model was further extended by Alfares and Al-Amir (2002) to include four main product categories: propylene, ethylene, synthesis gas and aromatics and their derivatives. They devised a non-linear objective function of production investment cost at different production levels and derived a linear representation of the function through piece-wise linear approximation. Al-Sharrah et al. (2001, 2002) presented MILP models that took sustainability and strategic technology selection into consideration. The models included a constraint to limit the selection of one technology to produce a chemical achieving a long term financial stability and an environmental consideration through a suitability objective. Sustainability was quantified by a health index of the chemicals and increasing profit was represented by the added value of each process in the network. This work was later extended by Al-Sharrah et al. (2003) with the aim of identifying long-range and short-range disturbances that affect planning of the petrochemical industry. Al-Sharrah et al. (2006) further developed their petrochemical planning framework into a multiobjective model accounting for economic gain

and risk from plant accidents. The above body of research did not account for parameter uncertainties.

The above discussion points out the importance of petrochemical network planning in process system engineering studies. In this chapter we develop a deterministic strategic planning model of a network of petrochemical processes. The problem is formulated as a mixed-integer linear programming (MILP) model with the objective of maximizing the added value of the overall petrochemical network.

5.3 Model Formulation

The optimization of petrochemical network design involves a broad range of aspects varying from economical and environmental analysis, strategic selection of processes and production capacities. The deterministic model presented in this study is slightly modified from that of Al-Sharrah et al. (2001, 2006). A set of CP number of chemicals involved in the operation of M_{pet} processes is assumed to be given. Let x_m^{Pet} be the annual level of production of process $m \in M_{pet}$, F_{cp}^{Pet} the amount of chemical $cp \in CP$ as a feedstock, and $\delta_{cp,m}$ the input-output coefficient matrix of material cp in process $m \in M_{pet}$, and $DPet_{cp}^{L}$ and $DPet_{cp}^{U}$ represent the lower and upper level of demand for product $cp \in CP$, respectively. Then, the material balance that governs the operation of the petrochemical network can be expressed as shown in constraints (5.1) and (5.2):

$$F_{cp}^{Pet} + \sum_{m \in M_{Pet}} \delta_{cp,m}\, x_m^{Pet} \geq DPet_{cp}^{L} \qquad \forall \; cp \in CP \tag{5.1}$$

$$F_{cp}^{Pet} + \sum_{m \in M_{Pet}} \delta_{cp,m}\, x_m^{Pet} \le D_{Pet}{}_{cp}^{U} \qquad \forall\ cp \in CP \tag{5.2}$$

For a given subset of chemicals where $cp \in CP$, these constraints control the production of different processes based on final products upper and lower demands of the petrochemical market. In constraint (5.3), defining the binary variables $y_{proc}{}_m^{Pet}$ for each process $m \in M_{pet}$ is required for the process selection requirement as $y_{proc}{}_m^{Pet}$ will equal 1 only if process *m* is selected or zero otherwise. Furthermore, if only process *m* is selected, its production level must be at least equal to the process minimum economic capacity B_m^L for each $m \in M_{pet}$, where K^U is a valid upper bound.. This can be written for each process m as follows:

$$B_m^L\, y_{proc}{}_m^{Pet} \le x_m^{Pet} \le K^U\, y_{proc}{}_m^{Pet} \qquad \forall\ m \in M_{Pet} \tag{5.3}$$

In the case where it is preferred or to choose only one process technology to produce a single chemical, constraints (5.4) and (5.5) can be included for each intermediate and product chemical type, respectively:

$$\sum_{cp \in CIP} y_{proc}{}_m^{Pet} \le 1 \qquad \forall\ m \in M_{Pet} \text{ that produces } cp \in CIP \text{ (intermediate)} \tag{5.4}$$

$$\sum_{cp \in CFP} y_{proc}{}_m^{Pet} \le 1 \qquad \forall\ m \in M_{Pet} \text{ that produces } cp \in CFP \text{ (final)} \tag{5.5}$$

Finally, we can specify limitations on the supply of feedstock S_{cp}^{Pet} for each chemical type cp though constraint (5.6) as follows:

$$F_{cp}^{Pet} \le S_{cp}^{Pet} \qquad \forall\ cp \in CP \tag{5.6}$$

The economic objective in the model can either be represented as operating cost minimization or added-value maximization. In the case of added-value maximization, products prices are subtracted from the cost of feedstocks for each process. If Pr_{cp}^{Pet} is the price of chemical cp, the added-value objective function can be represented as:

$$Max \quad \sum_{cp \in CP} \sum_{m \in M_{Pet}} Pr_{cp}^{Pet} \, \delta_{cp,m} \, x_m^{Pet} \tag{5.7}$$

5.4 Illustrative Case Study

The case study presented in this thesis is based on Al-Sharrah et al. (2006). The petrochemical network included 81 processes connecting the production and consumption of 65 chemicals. A simplified network of processes and chemicals included in the petrochemical network are given in Figure 5.1 and Table 5.1; respectively. The chemicals are classified according to their function as follows:

a) Primary raw material (*PR*)
b) Secondary raw material (*SR*)
c) Intermediate (*I*)
d) Primary final product (*PF*)
e) Secondary final product (*SF*)

PR chemicals are derived from petroleum and natural gas and other basic feedstocks, whereas the *SR* chemicals are those needed as additives or in small quantities.

Table 5.1 A list of chemicals included in the model

Chemical	Function	Chemical	Function
Acetaldehyde	SF+I	isopropyl alcohol	I
acetic acid	I+PF	methane	PR+SF
Acetone	PF	methanol	I
Acetylene	I	methyl acrylate	SR
acrylic fibers	PF	methyl methacrylate	SR
Acrylonitrile	I	naphtha	PR
acrylonitrile-butadiene-styrene	PF	*n*-butane	PR
Ammonia	PR	*n*-butylenes (1- and 2-)	PR
Benzene	SF+I	pentane	SR
Butadiene	I	Phenol	PR
butenes (mixed *n*-, iso-,-dienes, etc.)	SF+PR	polybutadiene rubber	SR
C-4 fraction (mixed butanes, -enes, etc.)	SF+PR	polystyrene (crystal grade)	I+PF
carbon dioxide	SR	polystyrene (expandable beds)	PF
carbon monoxide	I	Polystyrene (impact grade)	PF
Chlorine	PR	poly(vinyl acetate)	I
chlorobenzene	I	poly(vinyl alcohol)	SR
Coke	PR	poly(vinyl chloride)	PF
Cumene	I+PF	Propane	SF+PR
Ethane	PR	propylene (chemical grade)	SF+I
Etanol	I	propylene (refinery grade)	PR
ethyl benzene	I	propylene oxide	SF
Ethylene	SF+I	sodium carbonate	SR
ethylene dichloride	I	sodium hydroxide	SR
formic acid	SF	styrene	I
fuel gas	SF	sulfuric acid	I
fuel oil	SF+PR	sulfur	PR
gas oil	PR	synthesis gas 3:1	I
Gasoline	SF	synthesis gas 2:1	SF
hydrochloric acid	SR	toluene	PR+SF
Hydrogen	SR+SF	vinyl acetate	I+PF
hydrogen cyanide	I	vinyl chloride	I
hydrogen peroxide	I	xylene (mixed)	SR+SF

Also indicated the potential function of each chemical; PR= primary raw material, SR= secondary raw material, I= intermediate, PF= primary final product, SF= secondary final product.

The chemicals classified as *I* are those produced and consumed in the petrochemical network. Finally, the *PF* and *SF* chemicals are the selected final products by selected processes and the associated byproducts in the network; respectively.

The modeling system GAMS (Brooke et al., 1996) is used for setting up the optimization models. The computational tests were carried out on a Pentium M processor 2.13 GHz. The MILP model was solved using CPLEX (CPLEX Optimization Inc, 1993).

The model in this form is moderate in size and the solution indicated the selection of 22 processes out of the 81 processes proposed. The selected processes and their respective capacities are shown in Table 5.2. This case study represents an ideal situation where all parameters are known with certainty.

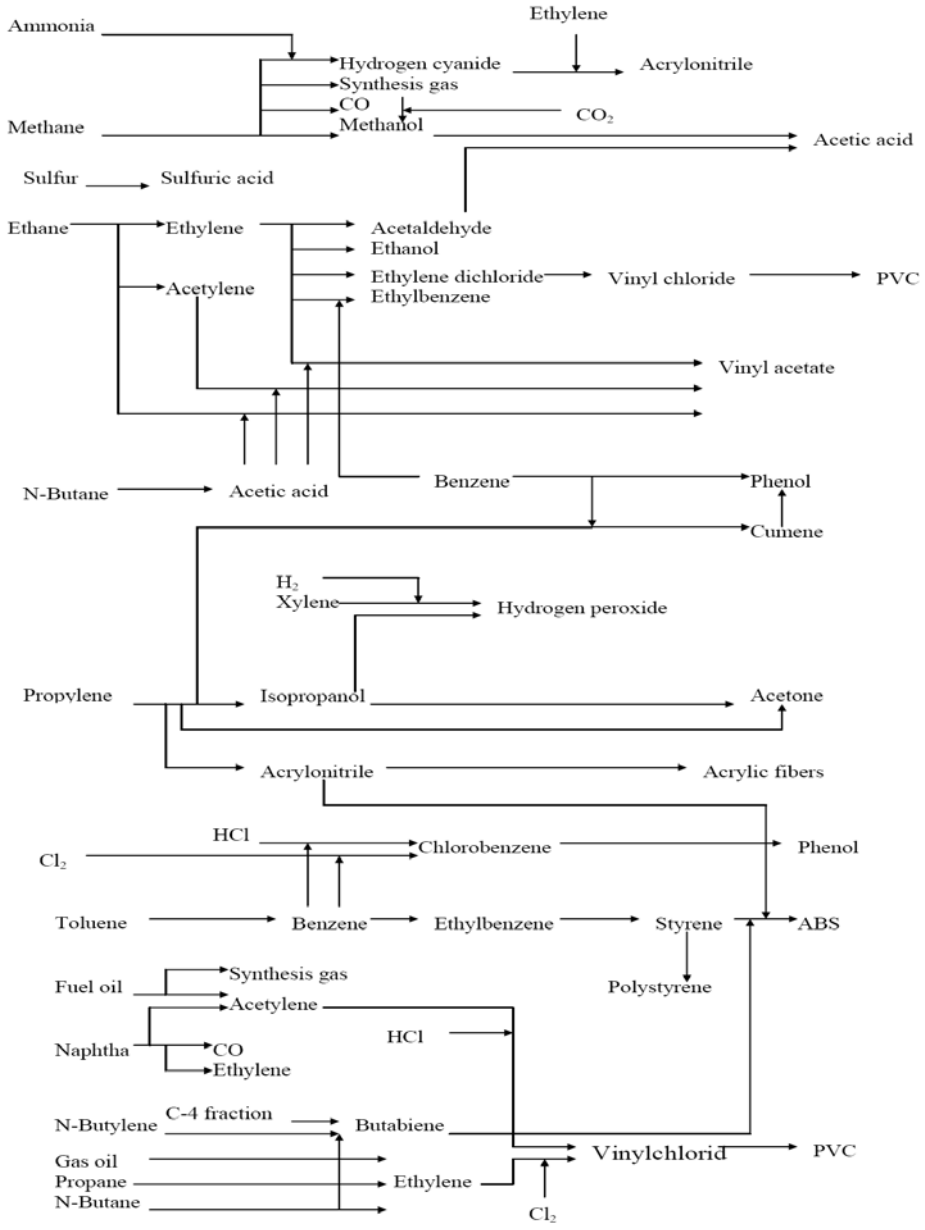

Figure 5.1 A simplified network of processes in the model.

The final petrochemical network suggests the use of lighter petroleum refining feedstocks. The petrochemical network mainly used ethane, propane, C-4 fractions (mixed butanes, -enes, etc.), pentane, and refinery grade propylene. In the case of lower lighter petroleum product availability, the network will suggest the use of steam cracking of naphtha or gas oil. This will be required in order to obtain the main petrochemical building blocks for the downstream processes that include ethylene and chemical grade propylene. The annual production benefit of the petrochemical network was found to be $ 2,202,268.

Table 5.2 Deterministic model solution

Process selected	Production Capacity (10^3 tons/yr)
acetaldehyde by the one-step oxidation from ethylene	1015.5
acetic acid by air oxidation of acetaldehyde	404.6
acetone by oxidation of propylene	169.8
acetylene by submerged flame process	179.8
acrylic fibers by batch suspension polymerization	246
acrylonitrile by cyanation/oxidation of ethylene	294.9
ABS by suspension/emulsion polymerization	386.9
benzene by hydrodealkylation of toluene	432.3
butadiene by extractive distillation	96.7
chlorobenzene by oxychlorination of benzene	73.0
cumene by the reaction of benzene and propylene	72.0
Ethylbenzene by the alkylation of benzene	458.8
ethylene by steam cracking of ethane-propane (50-50 wt%)	1068.3
hydrogen cyanide by the ammoxidation of methane	177.0
Phenol by dehydrochlorination of chlorobenzene	61.4
polystyrene (crystal grade) by bulk polymerization	66.8
polystyrene (expandable beads) by suspension polymerization	51.5
polystyrene (impact grade) by suspension polymerization	77.1
poly(vinyl chloride) by bulk polymerization	408.0
styrene from dehydrogenation of ethylbenzene	400.0
vinyl acetate from reaction of ethane and acetic acid	113.9
vinyl chloride by the hydrochlorination of acetylene	418.2

5.5 Conclusion

In this chapter we present an MILP deterministic planning model for the optimization of petrochemical network. The optimization model presents a tool that simplifies the process of decision-making for such large and complex petrochemical systems.

However, considering this type of high level strategic planning model, especially with the current volatile market environment and the continuous change in customer requirements, the impact of uncertainties is inevitable. In fact, ignoring uncertainty of key parameters in decision problems can yield non-optimal and infeasible decisions (Birge, 1995). For that reason, the scope of the following chapter is to extend the deterministic petrochemical planning model to account for uncertainties in model parameters and include the risk notion in decision-making using proper robust optimization techniques.

Chapter 6

Robust Optimization for Petrochemical Networks: Design under Uncertainty

6.1 Introduction

The discussion on planning under uncertainty in Chapter 4 and planning in the petrochemical networks in Chapter 5 underline the importance of modeling uncertainty and considering risk in process system engineering studies. In this chapter, we extend the model presented in Chapter 5 to address the strategic planning, design and optimization of a network of petrochemical processes under uncertainty and robust considerations. Robustness is analyzed based on both model robustness and solution robustness, where each measure is assigned a scaling factor to analyze the sensitivity of the refinery plan and integration network due to variations. For each term, a different scaling factor was used to analyze the sensitivity of the petrochemical network due to variations of each component. The stochastic model is formulated as a two-stage stochastic MILP problem whereas the robust optimization is formulated as an MINLP problem with nonlinearity arising from modeling the risk components. Both endogenous uncertainty, represented by uncertainty in the process yield and exogenous uncertainty, represented by uncertainty in raw material and product prices, and lower product market demand were considered. The concept of Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) are also investigated to numerically illustrate the value of including the randomness of the different model

parameters. The considerations of uncertainty in these parameters provided a more robust and practical analysis of the problem especially at a time when fluctuations in petroleum and petrochemical products prices and demands are soaring. For a literature review on planning of petrochemical networks, planning under uncertainty, and modeling risk, we refer the reader to Chapter 4 and 5.

The remainder of Chapter 6 is organized as follows. In the following section we will explain the proposed model formulation for the petrochemical network planning under uncertainty and with uncertainty and risk consideration, referred to as robust optimization. Then we will briefly explain the concept of value of information and stochastic solution, in section 6.3. In section 6.4, we will illustrate the performance of the model through an industrial case study. The chapter ends with concluding remarks in section 6.5.

6.2 Model Formulation

6.2.1 Two-Stage Stochastic Model

This formulation is an extension to the deterministic model presented in Chapter 5. In the previous chapter, all parameters of the model were assumed to be known with certainty. However, the current situation of fluctuating high petroleum crude oil and petrochemical product prices and demands is an indication of the high market and industry volatility. Acknowledging the shortcomings of deterministic models, parameter uncertainty is considered in the process yield $\delta_{cp,m}$, raw material and product prices Pr_{cp}^{Pet}, and lower product demand $D_{Pet}{}_{cp}^{L}$. The problem is formulated as a two-stage stochastic programming model. The uncertainty is considered through discrete distribution of the random parameters

with a finite number S of possible outcomes (scenarios) $\xi_k = (Pr_{cp,k}^{Pet}, \delta_{cp,m,k}, D_{Pet}{}_{cp,k}^{L})$ corresponding to a probability p_k. The formulation of the stochastic model is as follows:

$$\begin{aligned} Max \quad & \sum_{cp \in CP} \sum_{m \in M_{Pet}} \sum_{k \in N} p_k \, Pr_{cp,k}^{Pet} \, \delta_{cp,m,k} \, x_m^{Pet} \\ & - \sum_{cp \in CFP} \sum_{k \in N} p_k \, C_{cp}^{Pet+} \, V_{cp,k}^{Pet+} - \sum_{cp \in CFP} \sum_{k \in N} p_k \, C_{cp}^{Pet-} \, V_{cp,k}^{Pet-} \end{aligned} \tag{6.1}$$

Subject to

$$F_{cp}^{Pet} + \sum_{m \in M_{Pet}} \delta_{cp,m} \, x_m^{Pet} + V_{cp \in CFP,k}^{Pet+} - V_{cp,k}^{Pet-} = D_{Pet}{}_{cp,k}^{L} \quad \forall \; cp \in CP, \; k \in N \tag{6.2}$$

$$F_{cp}^{Pet} + \sum_{m \in M_{Pet}} \delta_{cp,m} \, x_m^{Pet} \le D_{Pet}{}_{cp \in CFP}^{U} \quad \forall \; cp \in CP, \; k \in N \tag{6.3}$$

$$B_m^L \, y_{proc}{}_m^{Pet} \le x_m^{Pet} \le K^U \, y_{proc}{}_m^{Pet} \quad \forall \; m \in M_{Pet} \tag{6.4}$$

$$\sum_{cp \in CIP} y_{proc}{}_m^{Pet} \le 1 \quad \forall \; m \in M_{Pet} \text{ that produces } cp \in CIP \text{ (intermediate)} \tag{6.5}$$

$$\sum_{cp \in CFP} y_{proc}{}_m^{Pet} \le 1 \quad \forall \; m \in M_{Pet} \text{ that produces } cp \in CFP \text{ (final)} \tag{6.6}$$

$$F_{cp}^{Pet} \le S_{cp}^{Pet} \quad \forall \; cp \in CP \tag{6.7}$$

The above formulation is a two-stage mixed-integer linear programming (MILP) model. The recourse variables $V_{cp,k}^{Pet+}$ and $V_{cp,k}^{Pet-}$ represent the shortfall and surplus for each random realization $k \in S$, respectively. These will compensate for the violations in constraints (6.2) and will be penalized in the objective function using the appropriate shortfall and surplus costs C_{cp}^{Pet+} and C_{cp}^{Pet-}, respectively. Uncertain parameters are assumed to follow a normal distribution for each outcome of the random realization ξ_k. The scenarios for all random

parameters are generated simultaneously. The recourse variables $V_{cp,k}^{Pet+}$ and $V_{cp,k}^{Pet-}$ in this formulation will compensate for deviations from the mean of the lower market demands $D_{Pet_{cp}}^{L}$ and process yield $\delta_{cp,m}$. In that way, the use of an independent recourse action and compensation for the violation in the constraint due to process yield uncertainty alone was avoided. Although this may not allow an explicit analysis for process yield uncertainty, it instead circumvents the complication of treating these types endogenous uncertainty.

6.2.2 Robust Optimization

The stochastic model with recourse in the previous section takes a decision merely based on first-stage and expected second-stage costs leading to an assumption that the decision-maker is risk-neutral (Sahinidis, 2004). In order to capture the concept of risk in stochastic programming, Mulvey et al. (1995) proposed the following amendment to the objective function:

$$Min_{x,y} \; c^T x + \mathrm{E}[Q(x,\xi(\omega))] + \lambda f(\omega, y)$$

where $\mathrm{E}[Q(x,\xi(\omega))]$ is the fixed recourse, f is a measure of variability (i.e. second moment) of the second-stage costs, and λ is a non-negative scalar representing risk tolerance. The representation through risk management using variance as a risk measure is often referred to as robust stochastic programming (Mulvey et al., 1995). This is also a typical risk measure following the Markowitz mean–variance (MV) model (Markowitz, 1952). The robustness is incorporated through the consideration of higher moments (variance) of the random parameter distribution ξ_k in the objective function and hence measuring the tradeoffs between mean value and variability.

In this study, operational risk was accounted for in terms of variance in both projected benefits, represented by first stage variables, and forecasted demand, represented by the recourse variables. The variability in the projected benefit represents the solution robustness where the model solution will remain close to optimal for all scenarios. On the other hand, variability of the recourse term represents the model robustness where the model solution will almost be feasible for all scenarios. This approach gives rise to a multiobjective analysis in which scaling factors are used to evaluate the sensitivity due to variations in each term. The projected benefits variation was scaled by θ_1 and deviation from forecasted demand was scaled by θ_2 where different values of θ_1 and θ_2 were used in order to observe the sensitivity of each term on the final petrochemical complex. The objective function with risk consideration can be written as follows:

$$\begin{aligned} Max \quad & \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} p_k\, Pr_{cp,k}^{Pet}\, \delta_{cp,m,k}\, x_m^{Pet} \\ & - \sum_{cp\in CFP}\sum_{k\in N} p_k\, C_{cp}^{Pet+}\, V_{cp,k}^{Pet+} - \sum_{cp\in CFP}\sum_{k\in N} p_k\, C_{cp}^{Pet-}\, V_{cp,k}^{Pet-} \\ & - \theta_1\sqrt{\text{var(Profit uncertainty)}} - \theta_2\sqrt{\text{var(Recourse uncertainty)}} \end{aligned} \tag{6.8}$$

Since the randomness in the profit uncertainty term is a multiplication of two random parameters, process yield $\delta_{cp,m,k}$ and chemical prices $Pr_{cp,k}^{Pet}$, its variance can be written based on the variance of a product of two variables x and y (Johnson and Tetley, 1955), i.e.:

$$\text{var}_{xy} = \text{var}_x\, \text{var}_y + \text{var}_x\, \mu_y + \text{var}_y\, \mu_x$$

where $\text{var}(x)$ and $\mu(x)$ represent the variance and mean value of a random number x; respectively. Hence, the objective function can be expressed as:

$$
\begin{aligned}
Max \quad & \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} p_k\, Pr_{cp,k}^{Pet}\, \delta_{cp,m,k}\, x_m^{Pet} \\
& - \sum_{cp\in CFP}\sum_{k\in N} p_k\, C_{cp}^{Pet+}\, V_{cp,k}^{Pet+} - \sum_{cp\in CFP}\sum_{k\in N} p_k\, C_{cp}^{Pet-}\, V_{cp,k}^{Pet-} \\
& -\theta_1 \sqrt{\begin{array}{l} \sum_{cp\in CFP}\sum_{m\in M_{Pet}} (x_m^{Pet})^2\, \mathrm{var}(\delta_{cp,m,k})\, \mathrm{var}(Pr_{cp,k}^{Pet}) \\ + \sum_{cp\in CFP}\sum_{m\in M_{Pet}} (x_m^{Pet})^2\, \mathrm{var}(\delta_{cp,m,k})\, \mu(Pr_{cp,k}^{Pet}) \\ + \sum_{cp\in CFP}\sum_{m\in M_{Pet}} (x_m^{Pet})^2\, \mu(\delta_{cp,m,k})\, \mathrm{var}(Pr_{cp,k}^{Pet}) \end{array}} \\
& -\theta_2 \sqrt{\sum_{cp\in CFP} \left[C_{cp}^{Pet+}\right]^2 \mathrm{var}(V_{cp,k}^{Pet+}) + \sum_{cp\in CFP} \left[C_{cp}^{Pet-}\right]^2 \mathrm{var}(V_{cp,k}^{Pet-})}
\end{aligned}
\tag{6.9}
$$

By expanding the mean and variance terms of $Pr_{cp,k}^{Pet}$, $\delta_{cp,m,k}$, $V_{cp,k}^{Pet+}$ and $V_{cp,k}^{Pet-}$, the objective function can be recast as:

$$
\begin{aligned}
Max \quad & \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} p_k\, Pr_{cp,k}^{Pet}\, \delta_{cp,m,k}\, x_m^{Pet} \\
& - \sum_{cp\in CFP}\sum_{k\in N} p_k\, C_{cp}^{Pet+}\, V_{cp,k}^{Pet+} - \sum_{cp\in CFP}\sum_{k\in N} p_k\, C_{cp}^{Pet-}\, V_{cp,k}^{Pet-} \\
& -\theta_1 \sqrt{\begin{array}{l} \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} (x_m^{Pet})^2\, p_k \left[\delta_{cp,m,k} - \sum_{k\in N} p_k\, \delta_{cp,m,k}\right]^2 \left[Pr_{cp,k}^{Pet} - \sum_{k\in N} p_k\, Pr_{cp,k}^{Pet}\right]^2 \\ + \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} (x_m^{Pet})^2\, p_k \left[\delta_{cp,m,k} - \sum_{k\in N} p_k\, \delta_{cp,m,k}\right]^2 \left(\sum_{k\in N} p_k\, Pr_{cp,k}^{Pet}\right) \\ + \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} (x_m^{Pet})^2\, p_k \left[Pr_{cp,k}^{Pet} - \sum_{k\in N} p_k Pr_{cp,k}^{Pet}\right]^2 \left(\sum_{k\in N} p_k\, \delta_{cp,m,k}\right) \end{array}} \\
& -\theta_2 \sqrt{\begin{array}{l} \sum_{cp\in CP} \left[C_{cp}^{Pet+}\right]^2 \sum_{k\in N} p_k \left[V_{cp,k}^{Pet+} - \sum_{k\in N} p_k\, V_{cp,k}^{Pet+}\right]^2 \\ + \sum_{cp\in CP} \left[C_{cp}^{Pet-}\right]^2 \sum_{k\in N} p_k \left[V_{cp,k}^{Pet-} - \sum_{k\in N} p_k\, V_{cp,k}^{Pet-}\right]^2 \end{array}}
\end{aligned}
\tag{6.10}
$$

In order to understand the effect of each term on the overall objective function of the petrochemical network, different values of θ_1 and θ_2 should be evaluated as will be shown in the illustrative case study.

6.3 Value to Information and Stochastic Solution

Since stochastic programming adds computational burden on practical problems, it is desirable to quantify the benefits of considering uncertainty. In order to address this point, there are generally two values of interest. One is *expected value of perfect information* (EVPI) which measures the maximum amount the decision maker is willing to pay in order to get accurate information on the future. The second is *value of stochastic solution* (VSS) which is the difference in the objective function between the solutions of mean value problem (replacing random events with their means) and the stochastic solution (SS). (Birge, 1982)

A solution based on perfect information would yield optimal first stage decisions for each realization of the random parameters ξ. Then the expected value of these decisions, known as "wait-and-see" (WS) can be written as (Madansky, 1960):

$$WS = E_{\xi}[Min\ z(x,\xi)]$$

However, since our objective is profit maximization, the expected value of perfect information (EVPI) can be calculated as:

$$EVPI = WS - SS \tag{6.11}$$

The other quantity of interest is the value of stochastic solution (VSS). In order to quantify it, we first need to solve the mean value problem, also referred to as the expected value problem (EV). This can be defined as $Min\ z(x, E[\xi])$ where $E[\xi] = \bar{\xi}$ (Birge, 1982). The solution of the EV problem provides the first stage decisions variables evaluated at expectation of the random realizations. The expectation of the EV problem, evaluated at different realization of the random parameters, is then defined as (Birge, 1982):

$$EEV = E_{\xi}[Min\ z(\bar{x}(\bar{\xi}), \xi)]$$

where $\bar{x}(\bar{\xi})$ is evaluated from the EV model, allowing the optimization problem to choose second stage variables with respect to ξ. Similarly since our objective is profit maximization, the value of stochastic solution can be expressed as:

$$VSS = SS - EEV \tag{6.12}$$

The value of stochastic solution can also be evaluated as the cost of ignoring uncertainty in the problem. These concepts will be evaluated in our case study.

6.4 Illustrative Case Study

A number of case studies were developed to demonstrate the performance of the optimization models and illustrate the effect of process yield, raw material and product prices, and lower product market demand variations. The case study in this chapter is based on Al-Sharrah et al. (2006) and is the same as the example presented in Chapter 5. The petrochemical network included 81 processes connecting the production and consumption of 65 chemicals which gave rise to 5265 uncertain process yield parameters. In addition, the model included 11

uncertain product demand parameters and 65 uncertain parameters representing raw materials and product prices. This gives a total of 5341 uncertain parameters which were modeled with a total number of 200 scenarios for each random parameter. Due to the high number of uncertain parameters and that fact that these type of data are generally stored in spreadsheets, all scenarios where generated in Excel spreadsheets using a pseudo random number generator. The input data was then imported to GAMS using the GAMS-Excel interface. All uncertain parameters were assumed to have a normal distribution. However, this assumption bears no restriction to the generality of the proposed modeling approach as other sampling distributions can be easily used instead.

The modeling system GAMS (Brooke et al., 1996) is used for setting up the optimization models. The computational tests were carried out on a Pentium M processor 2.13 GHz. The models were solved with DICOPT (Viswanathan & Grossmann, 1990). The NLP subproblems were solved with CONOPT2 (Drud, 1994), while the MILP master problems were solved with CPLEX (CPLEX Optimization Inc, 1993).

6.4.1 Solution of Stochastic Model

The two-stage mixed-integer stochastic program with recourse that includes a total number of 200 scenarios for each random parameter is considered in this section. All random parameters were assumed to follow a normal distribution and the scenarios for all random parameters were generated simultaneously. Therefore, the recourse variables account for the deviation from a given scenario as opposed to the deviation from a particular random number realization.

Table 6.1 shows the stochastic model solution for the petrochemical system. The solution indicated the selection of 22 processes with a slightly different configuration and production capacities from the deterministic case, Table 5.2. For example, acetic acid was produced by direct oxidation of *n*-butylenes instead of the air oxidation of acetaldehyde. Furthermore, ethylene was produced by pyrolysis of ethane instead of steam cracking of ethane-propane (50-50 wt%). These changes as well as the different production capacities obtained illustrate the effect of the uncertainty in process yield, raw material and product prices, and lower product demands. In fact, ignoring uncertainty of key parameters in decision problems can yield non-optimal and infeasible decisions (Birge, 1995). The annual profit of the petrochemical network studied under uncertainty was found to be $ 2,698,552.

Table 6.1 Stochastic model solution

Process selected	**Production Capacity (10^3 tons/yr)**
acetaldehyde by the one-step oxidation from ethylene	991.0
acetic acid by direct oxidation of *n*-butylenes	397.6
acetone by oxidation of propylene	169.6
acetylene by submerged flame process	179.7
acrylic fibers by batch suspension polymerization	245.8
acrylonitrile by cyanation/oxidation of ethylene	300.9
ABS by suspension/emulsion polymerization	419.6
benzene by hydrodealkylation of toluene	767.4
butadiene by extractive distillation	104.9
chlorobenzene by oxychlorination of benzene	146.0
cumene by the reaction of benzene and propylene	144.3
Ethylbenzene by the alkylation of benzene	692.8
ethylene by pyrolysis of ethane	1051.8
hydrogen cyanide by the ammoxidation of methane	180.6
Phenol by dehydrochlorination of chlorobenzene	122.7
polystyrene (crystal grade) by bulk polymerization	133.4
polystyrene (expandable beads) by suspension polymerization	102.8
polystyrene (impact grade) by suspension polymerization	154.1
poly(vinyl chloride) by bulk polymerization	407.6
styrene from ethylbenzene by hydroperoxide process	607.7
vinyl acetate from reaction of ethylene and acetic acid	113.8
vinyl chloride by the hydrochlorination of acetylene	417.8

However, in order to properly evaluate the added-value of including uncertainty of the problem parameters, we will investigate both the expected value of perfect information (EVPI) and the value of stochastic solution (VSS).

In order to evaluate the value of stochastic solution (VSS) we first solved the deterministic problem, as illustrated in the previous section, and fixed the petrochemical network and the production rate of the processes. We then solved the EEV problem by allowing the optimization problem to choose second stage variables with respect to the realization of the uncertain parameters ξ. From (6.12), the VSS is:

$$VSS = 2{,}698{,}552 - EEV$$
$$EEV = 2{,}184{,}930$$
$$VSS = 513{,}622$$

This indicates that the benefit of incorporating uncertainty in the different model parameters for the petrochemical network investment is $ 513,622. On the other hand, the expected value of perfect information (EVPI) can be evaluated by first finding the "wait-and-see" (WS) solution. The latter can be obtained by taking the expectation for the optimal first stage decisions evaluated at each realization ξ. From (6.11), the EVPI is:

$$EVPI = WS - 2{,}698{,}552$$
$$WS = 2{,}724{,}040$$
$$EVPI = 25{,}488$$

This implies that if it were possible to know the future realization of the demand, prices and yield perfectly, the profit would have been $2,724,040 instead of $2,698,552, yielding savings of $25,488. However, since acquiring perfect information is not viable, we will

merely consider the value of stochastic solution (SS) as the best result. These results show that the stochastic model provided an excellent solution as the objective function value was not too far from the result obtained by the WS solution.

However, as mentioned in the previous section, the stochastic model takes a decision based on first-stage and expected second-stage costs and hence does not account for a decision-maker risk behavior (risk-averse or risk taker). For this reason, a more realistic approach would consider higher moments where the tradeoff between the mean value and the variations of different scenarios is appropriately reflected.

6.4.2 Solution of Robust Model

Considering risk in terms of variations in both projected benefits and recourse variables provided a more robust analysis of the problem. As explained earlier, the problem will have a more robust solution as the results will remain close to optimal for all given scenarios through minimizing the variations of the projected benefit. On the other hand, the model will be more robust as minimizing the variations in the recourse variables leads to a model that is almost feasible for all the scenarios considered. In order to investigate the effect of each term on the original problem, the spectrum of results generated by varying the scaling factors must be explored. For this reason, the model was repeatedly solved for different values of θ_1 (profit variations) and θ_2 (recourse variables variations) in order to construct the efficient frontier plot of expected profit versus risk measured by standard deviation. Figures 6.1 illustrates the change in profit with different values of profit variations, denoted by θ_1, and recourse variables variations, denoted by θ_2. The graph shows the decline in expected profit as we penalize the variations in process yield, profit and demand by increasing the values of

θ_1 and θ_2. These values will depend on the policy adopted by the investor whether being risk-averse or risk taker and can be read directly from the efficient frontier plots. Figure 6.2 demonstrates the tradeoff between profit with risk, represented by the total standard deviation in prices and demand, with respect to different values of θ_1 and θ_2. Furthermore, it was found that the problem bears more sensitivity to variations in product prices as apposed to product demand and process yields for values of θ_1 and θ_2 that maintain the final petrochemical structure. As the values of θ_1 and θ_2 increase some processes became too risky to include in the petrochemical network and instead, importing some final chemicals became a more attractive alternative. This type of analysis requires accurate pricing structure of the local market under study as compared to the global market. In this study, however, we restricted the range of the variations of scaling parameters θ_1 and θ_2 to values that will maintain all processes obtained from the stochastic model. This approach was adopted as the objective of the study was to include all required processes that will meet a given demand.

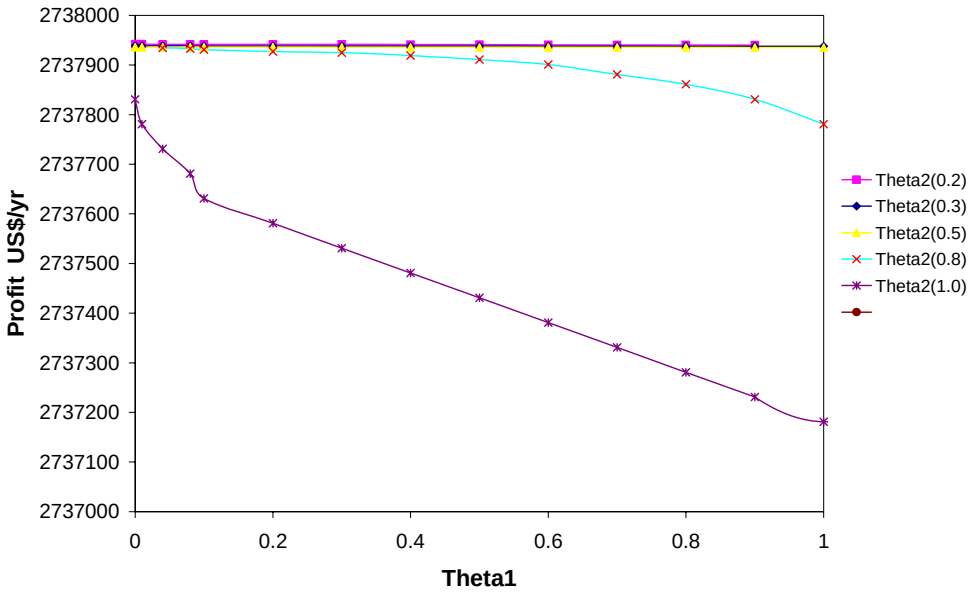

Figure 6.1 Profit variation with different values of θ_1 and θ_2.

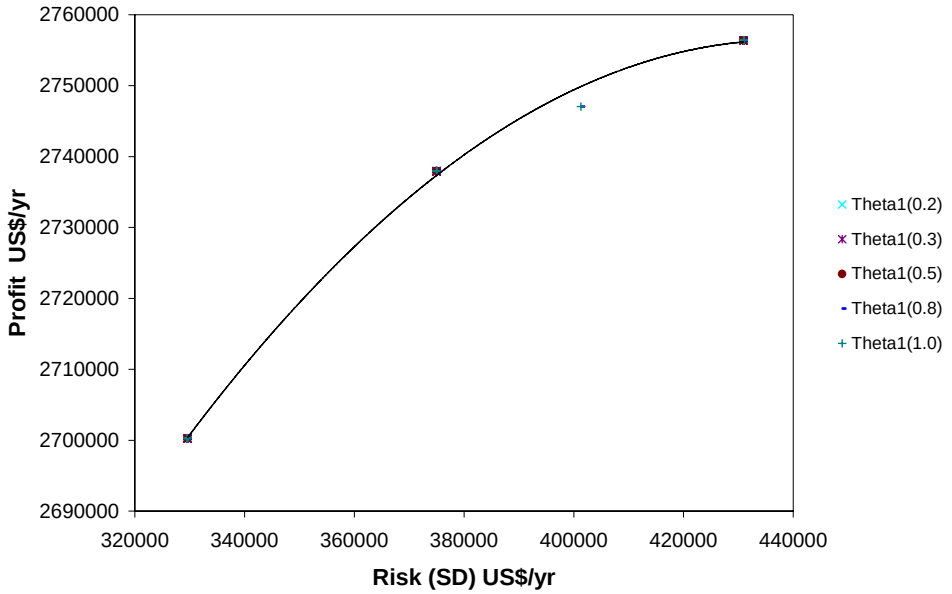

Figure 6.2 Tradeoff between profit and risk at different θ_2 values while varying θ_1.

6.5 Conclusion

A robust mixed-integer nonlinear programming model for maximizing profit in the design of petrochemical networks was presented. Uncertainty in process yield, raw material and product prices, and lower product market demand were considered. In addition, operational risk was accounted for in terms of variance in projected benefits, process yield and forecasted demand. Including these different sources of uncertainty in the problem as well as modeling risk provided a more robust analysis for this type of highly strategic planning application in the chemical industry. The proposed approach increased solution robustness and model robustness by incorporating penalty terms for both deviation from both projected benefits and recourse variables, respectively.

The results of the model studied under uncertainty and with risk consideration, as one can intuitively anticipate, yielded different petrochemical network configurations and plant capacities when compared to the deterministic model results. The concepts of Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) were introduced and numerically illustrated. The results obtained from the stochastic model provided good results as the objective function value was not too far from the results obtained using the wait-and-see approach. Furthermore, the study showed that the final petrochemical network bears more sensitivity to variations in product prices as apposed to variation in market demand and process yields when the values of θ_1 and θ_2 were selected to maintain the final petrochemical structure.

Chapter 7

Multisite Refinery and Petrochemical Network Design: Optimal Integration and Coordination

7.1 Introduction

In view of the current situation of high oil prices and the increasing consciousness and implementation of strict environmental regulations, petroleum refiners and petrochemical companies started seeking opportunities for mergers and integration. This is evident in the current projects around the world for building integrated refineries and the development of complex petrochemical industries that are aligned through advanced integration platforms. Figure 7.1 illustrates a typical refining and petrochemical industry supply chain. The realization of coordination and objective alignment benefits across the enterprise has been the main driver of such efforts (Sahinidis et al., 1989; Shah, 1998).

Despite the fact that petroleum refining and petrochemical companies have recently engaged in more integration projects, relatively little research in the open literature has been reported, mostly due to confidentiality reasons. Such concerns render the development of a systematic framework of network integration and coordination difficult. The studies published in the open literature were mainly developed by consulting and design firms, as well as the operating companies, and generally lack a structured methodology for evaluating the projects feasibility. Just to mention a few of the studies published, Swaty (2002) studied

the possibility of integrating a refinery and an ethylene plant through the exchange of process intermediate streams. The analysis was based on a linear programming model for each plant and profit marginal analysis of possible intermediate plant exchange. The study was implemented on a real life application in western Japan. Gonzalo et al. (2004) highlighted the benefits of refining and petrochemical integration. They discussed a project dealing with the installation of a hydrocracker in Repsol's Refinery in Spain and how it improved the overall synergy between the refinery and a stream cracker plant.

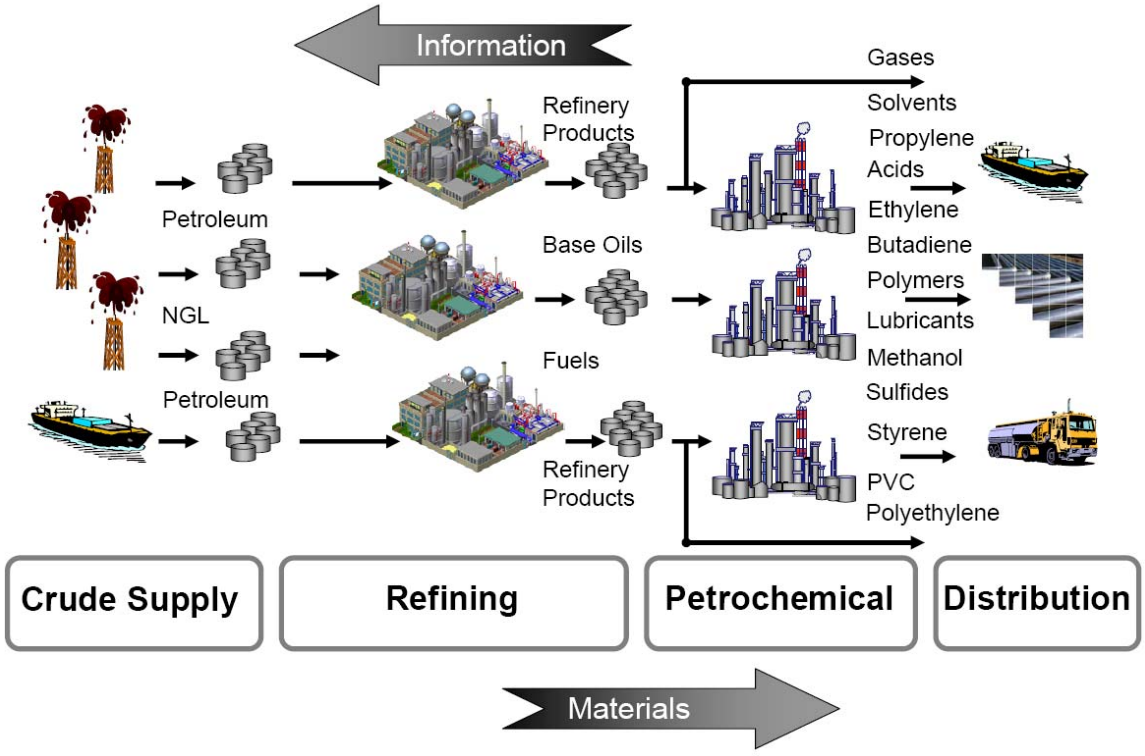

Figure 7.1 Refinery and petrochemical industry supply chain.

In the academic arena, Sadhukhan et al. (2004) developed an analytical flowsheet optimization method for applications in the petroleum refining and petrochemical industry. The proposed methodology consisted of three main steps: market integration, facility

network optimization through economic margin analysis and load shifting, and elimination of less profitable processes. They demonstrated their method on two case studies: a single site refinery and a petrochemical complex. Li et al. (2006) proposed a Linear Programming (LP) model for the integration of a refinery and an ethylene cracker. They evaluated different schemes iteratively for different crude types to optimize the refinery and ethylene cracker operations. The best scheme was selected based on the highest profit from the cases studied. More recently, Kuo and Chang (2008) developed a short term multi-period planning model for a benzene-toluene-xylene (BTX) complex. They modeled the system as a mixed integer linear programming (MILP) model with binary variables mainly for mode switching and inventory control (backlog and surplus indication). They divided the processing units into two sets, 1) reaction processes: reforming, isomerization units and tatory units, and 2) separation processes: aromatics extraction units, xylene fractionation units and the parex units. Optimization of the other refinery units, blending levels and olefin cracking process were not considered. The decisions in their study mainly included the optimal throughput and operation mode of each production unit, inventory levels and feedstock supplies. For more details on strategic multisite planning studies, multisite refinery optimization, and petrochemical industry planning the interested reader is referred to the previous chapters and the references given herein.

Petroleum refining and petrochemical plants integration is gaining a great deal of interest with the realization of coordination and vertical integration benefits. Previous research in the field assumed either no limitations on refinery feedstock availability for the petrochemical planning problem or fixed the refinery production levels assuming an optimal operation. However, in this chapter we present a mathematical model for the determination of the

optimal integration and coordination strategy for a refinery network and synthesize the optimal petrochemical network required to satisfy a given demand from any set of available technologies. Therefore, achieving a global optimal production strategy by allowing appropriate trade offs between the refinery and the downstream petrochemical markets. The refinery and petrochemical systems were modeled as MILP problems that will also lead to overall refinery and petrochemical process production levels and detailed blending levels at each refinery site. The objective function is a minimization of the annualized cost over a given time horizon among the refineries by improving the coordination and utilization of excess capacities in each facility and maximization of the added value in the petrochemical system. Expansion requirements to improve production flexibility and reliability in the refineries are also considered.

The remainder of Chapter 7 is organized as follows. In the following section, we explain the problem statement of the petroleum refinery and petrochemical integration. Then, we discuss the proposed model formulation in section 7.3. In section 7.4, we illustrate the performance of the model through an industrial-scale case study. The chapter ends with some concluding remarks in section 7.5.

7.2 Problem Statement

The optimization of refining and petrochemical processes involves a wide range of aspects varying from economical analysis and strategic expansions to crude oil selection, process levels targets, operating modes, etc. The focus of this study is to develop a mathematical programming tool for the simultaneous design of an integrated network of refineries and petrochemical processes. On the refinery side, the model provides the optimal network

integration between the refineries, process expansion requirements, operating policy based on different feedstock combination alternatives, process levels and operating modes. On the petrochemical side, the model establishes the design of an optimal petrochemical process network from a range of process technologies to satisfy a given demand. The simultaneous network design and optimization of the refining and petrochemical industry provides appropriate means for improving the coordination across the industrial system and is prone to develop an overall optimal production strategy across the petroleum chain.

The general problem under study can be defined as follows:

A set of refinery products $cfr \in CFR$ produced at multiple refinery sites $i \in I$ and a set of petrochemical products $cp \in CFP$ is given. Each refinery consists of different production units $m \in M_{Ref}$ that can operate at different modes $p \in P$ while a set of wide range petrochemical and chemical process technologies $m \in M_{Pef}$ is available for selection. Furthermore, different crude oil slates $cr \in CR$ are available and given. The petrochemical network selects its feedstock from three main sources; namely, refinery intermediate streams $Fi^{Pet}_{cr,cir,i}$ of an intermediate product $cir \in RPI$, refinery final products $Ff^{Pet}_{cr,cfr,i}$ of a final product $cfr \in RPF$, and non-refinery streams Fn^{Pet}_{cp} of a chemical $cp \in NRF$. The process network across the refineries and petrochemical system is connected in a finite number of ways. An integration superstructure between the refinery processes is defined in order to allow exchanging intermediate streams. Market product prices, operating cost at each refinery and petrochemical system, as well as product demands are assumed to be known.

The problem consists of determining the optimal integration and coordination strategy for the overall refinery network and designing the optimal petrochemical network required to satisfy a given demand from the available process technologies. The proposed approach will also provide overall refinery and petrochemical process production levels and detailed blending levels at each refinery site. The objective function is a minimization of the annualized cost over a given time horizon among the refineries by improving the coordination and utilization of excess capacities in each facility and maximization of the added value in the petrochemical system. Expansion requirements to improve production flexibility and reliability in the refineries are also considered.

For all refinery and petrochemical processes within the network we assume that all material balances are expressed in terms of linear yield vectors. Even though this might sound restrictive as most if not all refinery and petrochemical processes are inherently nonlinear, this practice is commonly applied with such large scale systems. Moreover, the decisions in this study are of a strategic level in which such linear formulation is adequate to address the required level of details involved at this stage. It is also assumed that processes have fixed capacities and the operating cost of each process and production mode is proportional to the process inlet flow. In the case of refinery product blending, quality blending indices are used to maintain model linearity. It is also assumed that all products that are in excess of the local demand can be exported to a global market. Piping and pumping installation costs to transport refinery intermediate streams between the different refinery sites as well as the operating costs of the new system are lumped into one fixed-charge cost. All costs are discounted over a 20 years time horizon and with an interest rate of 7%. No inventories will be considered since the model is addressing strategic decisions

which usually cover a long period of time. We also assume perfect mixing in the refineries and that the properties of each crude oil slate are decided by specific key components.

7.3 Model Formulation

The proposed formulation addresses the problem of simultaneous design of an integrated network of refineries and petrochemical processes. The proposed model is based on the formulations proposed in this dissertation. All material balances are carried out on a mass basis with the exception of refinery quality constraints of properties that only blend by volume where volumetric flowrates are used instead. The model is formulated as follows:

$$
\begin{aligned}
Min \quad & \sum_{cr\in CR}\sum_{i\in I} CrCost_{cr}\; S^{Ref}_{cr,i} \\
& + \sum_{p\in P} OpCost_{p} \sum_{cr\in CR}\sum_{i\in I} z_{cr,p,i} \\
& + \sum_{cir\in CIR}\sum_{i\in I}\sum_{i'\in I} InCost_{i,i'}\; ypipe^{Ref}_{cir,i,i'} \\
& + \sum_{i\in I}\sum_{m\in M_{Ref}}\sum_{s\in S} InCost_{m,s}\; yexp^{Ref}_{m,i,s} \qquad \text{where } i \neq i' \\
& - \sum_{cfr\in PEX}\sum_{i\in I} Pr^{Ref}_{cfr}\; e^{Ref}_{cfr,i} \\
& - \sum_{cp\in CP}\sum_{m\in M_{Pet}} Pr^{Pet}_{cp}\; \delta_{cp,m}\; x^{Pet}_{m}
\end{aligned}
\tag{7.1}
$$

Subject to

$$
z_{cr,p,i} = S^{Ref}_{cr,i} \qquad \forall\ cr \in CR,\ i \in I \qquad \text{where } p \in P' = \{\text{Set of CDU processes } \forall \text{ plant i}\} \tag{7.2}
$$

$$\sum_{p\in P}\alpha_{cr,cir,i,p}\ z_{cr,p,i}+\sum_{i'\in I}\sum_{p\in P}\xi_{cr,cir,i',p,i}\ xi^{Ref}_{cr,cir,i',p,i}-Fi^{Pet}_{cr,cir\in RPI,i}$$
$$-\sum_{i'\in I}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'}-\sum_{cfr\in CFR}w_{cr,cir,cfr,i}-\sum_{rf\in FUEL}w_{cr,cir,rf,i}=0 \qquad \begin{array}{l}\forall\ cr\in CR,\\ cir\in CIR,\\ i'\&i\in I\\ \text{where}\quad i\neq i'\end{array} \qquad (7.3)$$

$$\sum_{cr\in CR}\sum_{cir\in CB}w_{cr,cir,cfr,i}-\sum_{cr\in CR}\sum_{rf\in FUEL}w_{cr,cfr,rf,i}-\sum_{cr\in CR}Ff^{Pet}_{cr,cfr\in RPF,i}=x^{Ref}_{cfr,i} \qquad \begin{array}{l}\forall\\ cfr\in CFR,\\ i\in I\end{array} \qquad (7.4)$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}}=xv^{Ref}_{cfr,i} \qquad \forall\ \begin{array}{l}cfr\in CFR,\\ i\in I\end{array} \qquad (7.5)$$

$$\sum_{cir\in FUEL}cv_{rf,cir,i}\ w_{cr,cir,rf,i}+\sum_{cfr\in FUEL}w_{cr,cfr,rf,i}-\sum_{p\in P}\beta_{cr,rf,i,p}\ z_{cr,p,i}=0 \qquad \begin{array}{l}\forall\\ cr\in CR,\\ rf\in FUEL,\\ i\in I\end{array} \qquad (7.6)$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\left(\begin{array}{l}att_{cr,cir,q\in Qv}\ \dfrac{w_{cr,cir,cfr,i}}{sg_{cr,cir}}+att_{cr,cir,q\in Qw}\\ \left[w_{cr,cir,cfr,i}-\sum_{rf\in FUEL}w_{cr,cfr,rf,i}-\sum_{cr\in CR}Ff^{Pet}_{cr,cfr\in RPF,i}\right]\end{array}\right)$$
$$\geq q^{L}_{cfr,q\in Qv}\ xv^{Ref}_{cfr,i}+q^{L}_{cfr,q\in Qw}\ x^{Ref}_{cfr,i} \qquad \begin{array}{l}\forall\\ cfr\in CFR,\\ q=\{Qw,Qv\},\\ i\in I\end{array} \qquad (7.7)$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\left(\begin{array}{l}att_{cr,cir,q\in Qv}\ \dfrac{w_{cr,cir,cfr,i}}{sg_{cr,cir}}+att_{cr,cir,q\in Qw}\\ \left[w_{cr,cir,cfr,i}-\sum_{rf\in FUEL}w_{cr,cfr,rf,i}-\sum_{cr\in CR}Ff^{Pet}_{cr,cfr\in RPF,i}\right]\end{array}\right)$$
$$\leq q^{U}_{cfr,q\in Qv}\ xv^{Ref}_{cfr,i}+q^{U}_{cfr,q\in Qw}\ x^{Ref}_{cfr,i} \qquad \begin{array}{l}\forall\\ cfr\in CFR,\\ q=\{Qw,Qv\},\\ i\in I\end{array} \qquad (7.8)$$

$$MinC_{m,i}\leq\sum_{p\in P}\gamma_{m,p}\sum_{cr\in CR}z_{cr,p,i}\leq MaxC_{m,i}+\sum_{s\in S}AddC_{m,i,s}\ yexp^{Ref}_{m,i,s} \qquad \forall\ m\in M_{Ref},i\in I \qquad (7.9)$$

$$\sum_{cr\in CR}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'} \le F^{U}_{cir,i,i'}\ y_{pipe}{}^{Ref}_{cir,i,i'} \qquad \forall\ cir\in CIR, i' \,\&\, i\in I \text{ where } i\neq i' \qquad (7.10)$$

$$\sum_{i\in I}\left(x^{Ref}_{cfr,i} - e^{Ref}_{cfr',i}\right) \ge D_{Ref_{cfr}} \qquad \forall\ cfr\ \&\ cfr' \text{ where } cfr\in CFR, cfr'\in PEX \qquad (7.11)$$

$$IM^{L}_{cr} \le \sum_{i\in I} S^{Ref}_{cr,i} \le IM^{U}_{cr} \qquad \forall\ cr\in CR \qquad (7.12)$$

$$Fn^{Pet}_{cp\in NRF} + \sum_{i\in I}\sum_{cr\in CR} Fi^{Pet}_{cr,cp\in RPI,i} + \sum_{i\in I}\sum_{cr\in CR} Ff^{Pet}_{cr,cp\in RPF,i} + \sum_{m\in M_{Pet}} \delta_{cp,m}\ x^{Pet}_{m} \ge D_{Pet}{}^{L}_{cp\in CFP} \qquad \forall\ cp\in CP \qquad (7.13)$$

$$Fn^{Pet}_{cp\in NRF} + \sum_{i\in I}\sum_{cr\in CR} Fi^{Pet}_{cr,cp\in RPI,i} + \sum_{i\in I}\sum_{cr\in CR} Ff^{Pet}_{cr,cp\in RPF,i} + \sum_{m\in M_{Pet}} \delta_{cp,m}\ x^{Pet}_{m} \le D_{Pet}{}^{U}_{cp\in CFP} \qquad \forall\ cp\in CP \qquad (7.14)$$

$$B^{L}_{m}\ y_{proc}{}^{Pet}_{m} \le x^{Pet}_{m} \le K^{U}\ y_{proc}{}^{Pet}_{m} \qquad \forall\ m\in M_{Pet} \qquad (7.15)$$

$$\sum_{cp\in CIP} y_{proc}{}^{Pet}_{m} \le 1 \qquad \forall\ m\in M_{Pet} \text{ that produces } cp\in CIP \qquad (7.16)$$

$$\sum_{cp\in CFP} y_{proc}{}^{Pet}_{m} \le 1 \qquad \forall\ m\in M_{Pet} \text{ that produces } cp\in CFP \qquad (7.17)$$

$$Fn^{Pet}_{cp} \le S^{Pet}_{cp} \qquad \forall\ cp\in NRF \qquad (7.18)$$

The above objective function (7.1) represents a minimization of the annualized cost which consists of crude oil cost, refineries operating cost, refineries intermediate exchange piping cost, refinery production system expansion cost, less the refinery export revenue and added value by the petrochemical processes. The operating cost of each refinery process is assumed to be proportional to the process inlet flow and is expressed on a yearly basis. Inequality (7.2) corresponds to each refinery raw materials balance where throughput to each distillation unit $p \in P'$ at plant $i \in I$ from each crude type $cr \in CR$ is equal to the available supply $S_{cr,i}^{Ref}$. Constraint (7.3) represents the intermediate material balances within and across the refineries where the coefficient $\alpha_{cr,cir,i,p}$ can assume either a positive sign if it is an input to a unit or a negative sign if it is an output from a unit. The multirefinery integration matrix $\xi_{cr,cir,i,p,i'}$ accounts for all possible alternatives of connecting intermediate streams $cir \in CIR$ of crude $cr \in CR$ from refinery $i \in I$ to process $p \in P$ in plant $i' \in I'$. Variable $xi_{cr,cir,i,p,i'}^{Ref}$ represents the transshipment flowrate of crude $cr \in CR$, of intermediate $cir \in CIR$ from plant $i \in I$ to process $p \in P$ at plant $i' \in I$. Constraint (7.3) also considers the petrochemical network feedstock from the refinery intermediate streams $Fi_{cr,cir,i}^{Pet}$ of each intermediate product $cir \in RPI$. The material balance of final products in each refinery is expressed as the difference between flowrates from intermediate steams $w_{cr,cir,cfr,i}$ for each $cir \in CIR$ that contribute to the final product pool and intermediate streams that contribute to the fuel system $w_{cr,cfr,rf,i}$ for each $rf \in FUEL$ less the refinery final products $Ff_{cr,cfr,i}^{Pet}$ for each $cfr \in RPF$ that are fed to the petrochemical network as shown in constraint (7.4). In constraint (7.5) we convert the mass flowrate to volumetric flowrate by dividing it by the

specific gravity $sg_{cr,cir}$ of each crude type $cr \in CR$ and intermediate stream $cir \in CB$. This is needed in order to express the quality attributes that blend by volume in blending pools. Constraint (7.6) is the fuel system material balance where the term $cv_{rf,cir,i}$ represents the caloric value equivalent for each intermediate $cir \in CB$ used in the fuel system at plant $i \in I$. The fuel production system can either consist of a single or combination of intermediates $w_{cr,cir,rf,i}$ and products $w_{cr,cfr,rf,i}$. The matrix $\beta_{cr,rf,i,p}$ corresponds to the consumption of each processing unit $p \in P$ at plant $i \in I$ as a percentage of unit throughput. Constraints (7.7) and (7.8), respectively, represent lower and upper bounds on refinery quality constraints for all refinery products that either blend by mass $q \in Q_w$ or by volume $q \in Q_v$. Constraint (7.9) represents the maximum and minimum allowable flowrate to each processing unit. The coefficient $\gamma_{m,p}$ is a zero-one matrix for the assignment of production unit $m \in M_{Ref}$ to process operating mode $p \in P$. The term $AddC_{m,i,s}$ accounts for the additional refinery expansion capacity of each production unit $m \in M_{Ref}$ at refinery $i \in I$ for a specific expansion size $s \in S$. In this formulation, we only allow the addition of predetermined capacities whose pricing can be acquired a priori through design companies' quotations. The integer variable $yexp^{Ref}_{m,i,s}$ represents the decision of expanding a production unit and it can take a value of one if the unit expansion is required or zero otherwise. Constraint (7.10) sets an upper bound on intermediate streams flowrates between the different refineries. The integer variable $ypipe^{Ref}_{cir,i,i'}$ represents the decision of exchanging intermediate products between the refineries and takes on the value of one if the commodity is transferred from plant $i \in I$ to plant $i' \in I$ or zero otherwise, where $i \neq i'$. When an intermediate stream is selected to be

exchanged between two refineries, its flowrate must be below the transferring pipeline capacity $F^{U}_{cir,i,i'}$. Constraint (7.11) stipulates that the final products from each refinery $x^{Ref}_{cfr,i}$ less the amount exported $e^{Ref}_{cfr',i}$ for each exportable product $cfr' \in PEX$ from each plant $i \in I$ must satisfy the domestic demand $D_{Ref_{cfr}}$. Resources are limited by constraint (7.12) which imposes upper and lower bounds on the available feedstock $cr \in CR$ to the refineries.

Constraints (7.13) and (7.14) represent the material balance that governs the operation of the petrochemical system. The variable x^{Pet}_{m} represents the annual level of production of process $m \in M_{pet}$ where $\delta_{cp,m}$ is the input-output coefficient matrix of material cp in process $m \in M_{pet}$.The petrochemical network receives its feed from potentially three main sources. These are, 1) refinery intermediate streams $Fi^{Pet}_{cr,cir,i}$ of an intermediate product $cir \in RPI$, 2) refinery final products $Ff^{Pet}_{cr,cfr,i}$ of a final product $cfr \in RPF$, and 3) non-refinery streams Fn^{Pet}_{cp} of a chemical $cp \in NRF$. For a given subset of chemicals $cp \in CP$, the proposed model selects the feed types, quantity and network configuration based on the final chemical and petrochemical lower and upper product demand $D_{Pet^{L}_{cp}}$ and $D_{Pet^{U}_{cp}}$ for each $cp \in CFP$, respectively. In constraint (7.15), defining a binary variable $y_{proc}{}^{Pet}_{m}$ for each process $m \in M_{pet}$ is required for the process selection requirement as $y_{proc}{}^{Pet}_{m}$ will equal 1 only if process m is selected or zero otherwise. Furthermore, if only process m is selected, its production level must be at least equal to the process minimum economic capacity B^{L}_{m} for each $m \in M_{pet}$, where K^{U} is a valid upper bound. In the case where it is preferred to choose only one process technology to produce a chemical, constraints (7.16) and (7.17) can be

included for each intermediate product $cp \in CIP$ and final product $cp \in CFP$, respectively. Finally, we can specify limitations on the supply of feedstock Fn_{cp}^{Pet} for each chemical type $cp \in NRF$ though constraint (7.18). Bear in mind that the limitations on the refinery intermediate product $Fi_{cr,cir,i}^{Pet}$ and final product $Ff_{cr,cfr,i}^{Pet}$ that are fed to the petrochemical network are dictated by the model based on both refinery and petrochemical demand and price structure.

7.4 Illustrative Case Study

In this section we demonstrate the performance of the proposed model on an industrial-scale case study. Instead of considering the full scale petrochemical network which may have limited application, we consider a special case of the integration problem. Although the proposed formulation covers the full scale refinery network and petrochemical systems, the case study will consider the integration of a petrochemical complex for the production of polyvinyl chloride (PVC) with a multirefinery network. PVC is one of the major ethylene derivatives that has many important applications and uses including pipe fittings, automobile bumpers, toys, bottles and many others (Rudd et al., 1981).

Direct integration of refining and ethylene cracking is considered as the essential building block in achieving the total petrochemical integration (Joly et al., 2002; Li et al., 2006). This problem has received more attention lately due to soaring motor gasoline prices and the directly related prices of ethylene feedstocks (Lippe, 2007). This kind of volatility in prices has prompted a shift in ethylene feedstock selection and economics to either lighter or heavier refinery product slates (Lippe, 2008). Shifting from one feedstock to another will

mainly depend on the market price structure and demand for refinery products. Some researchers believe that the tendency of ethylene feedstock shift would mainly be towards heavier refinery streams including heavy and vacuum gas oils due to the diminishing reserves of sweet crudes and decreasing demand of heavy fraction fuels (Singh et al., 2005; Van Geem et al., 2008). This change in ethylene feedstock selection and the direct effect on the refinery products requires adequate decision making and analysis that takes into account both refining and petrochemical markets.

Table 7.1 Major refinery network capacity constraints

Production Capacity	**Higher limit (10^3 ton/yr)**		
	R1	R2	R3
Distillation	45000.	12000.0	9900.0
Reforming	700.0	2000.0	1800.0
Isomerization	200.0	-	450.0
Fluid catalytic cracker	800.0	1400.0	-
Hydrocracker	-	1800.0	2400.0
Delayed coker	-	-	1800
Des gas oil	1300.0	3000.0	2400.0
Des cycle gas oil	200.0	750.0	-
Des ATK	-	1200.0	1680.0
Des Distillates	-	-	450.0
Crude availability			
Arabian Light		31200.0	
Local Demand			
LPG		432.0	
LN		-	
PG98		540.0	
PG95		4440.0	
JP4		2340.0	
GO6		4920.0	
ATK		1800.0	
HFO		200.0	
Diesel		400.0	
Coke		300.0	

In the case study, we consider the planning for three complex refineries by which we demonstrate the performance of our model in devising an overall production plan as well as

an integration strategy among the refineries. The state equipment network (SEN) representation for the overall topology of the refineries network is given in Figure 7.2.

The atmospheric crude unit separates crude oil into several fractions including LPG, naphtha, kerosene, gas oil and residues. The heavy residues are then sent to the vacuum unit where they are further separated into vacuum gas oil and vacuum residues. Depending on the production targets, different processing and treatment processes are applied to the crude fractions. In this example, the naphtha is further separated into heavy and light naphtha. Heavy naphtha is sent to the catalytic reformer unit to produce high octane reformates for gasoline blending and light naphtha is sent to the light naphtha pool and to an isomerization unit to produce isomerate for gasoline blending too, as in refineries 2&3. The middle distillates are combined with other similar intermediate streams and sent for hydrotreating and then for blending to produce jet fuels and gas oils. Atmospheric and vacuum gas oils are further treated by catalytic cracking, as in refinery 2, or by hydrocracking, as in refinery 3, or by both, as in refinery 1, to increase the gasoline and distillate yields. In refinery 3, vacuum residues are further treated using coking and thermal processes to increase light products yields. The final products of the three refineries network consists of liquefied petroleum gas (LPG), light naphtha (LT), two grades of gasoline (PG98 and PG95), No. 4 jet fuel (JP4), military jet fuel (ATKP), No.6 gas oil (GO6), diesel fuel (Diesel), heating fuel oil (HFO), and petroleum coke (coke). The major capacity constraints for the refinery network are given in Table 7.1. Furthermore, the three refineries are assumed to be in one industrial area, which is a common situation in many locations around the world, and are coordinated through a main headquarter sharing the feedstock supply. The cost parameters for pipelines installation were calculated as cost per distance between the refineries, and then multiplied by the required

pipe length in order to connect any two refineries. The pipeline diameter considered in all cases was 8 inches.

The petrochemical complex for the production of PVC starts with the production of ethylene from the refineries feedstocks. The main feedstocks to the ethylene plant in our study are light naphtha (LN) and gas oil (GO). The selection of the feedstocks and hence the process technologies are decided based on the optimal balance and trade-off between the refinery and petrochemical markets. The process technologies considered in this study for the production of PVC are list in Table 7.2. The overall topology of all petrochemical technologies for the PVC production is shown in Figure 7.3.

From the refinery side, the proposed model will provide the optimal network integration between the refineries, process expansion requirements, operating policy based on different feedstock combination alternatives, process levels and operating modes. On the petrochemical side, the model will establish the design of an optimal petrochemical process network for the production of PVC from the range of process technologies and feedstocks available to satisfy a given demand. This problem was formulated as an MILP with the overall objective of minimizing total annualized cost of the refinery and maximizing the added value from the PVC petrochemical network. Maximizing the added value of the petrochemical network is appropriate since the feedstocks costs contribute to the majority of the total cost. For instance, the feedstock cost of ethylene plant contributes to more than 87% of the total cost when naphtha is used and 84% and 74% when propane and ethane are used, respectively (NBK MENA Equity Research, 2007).

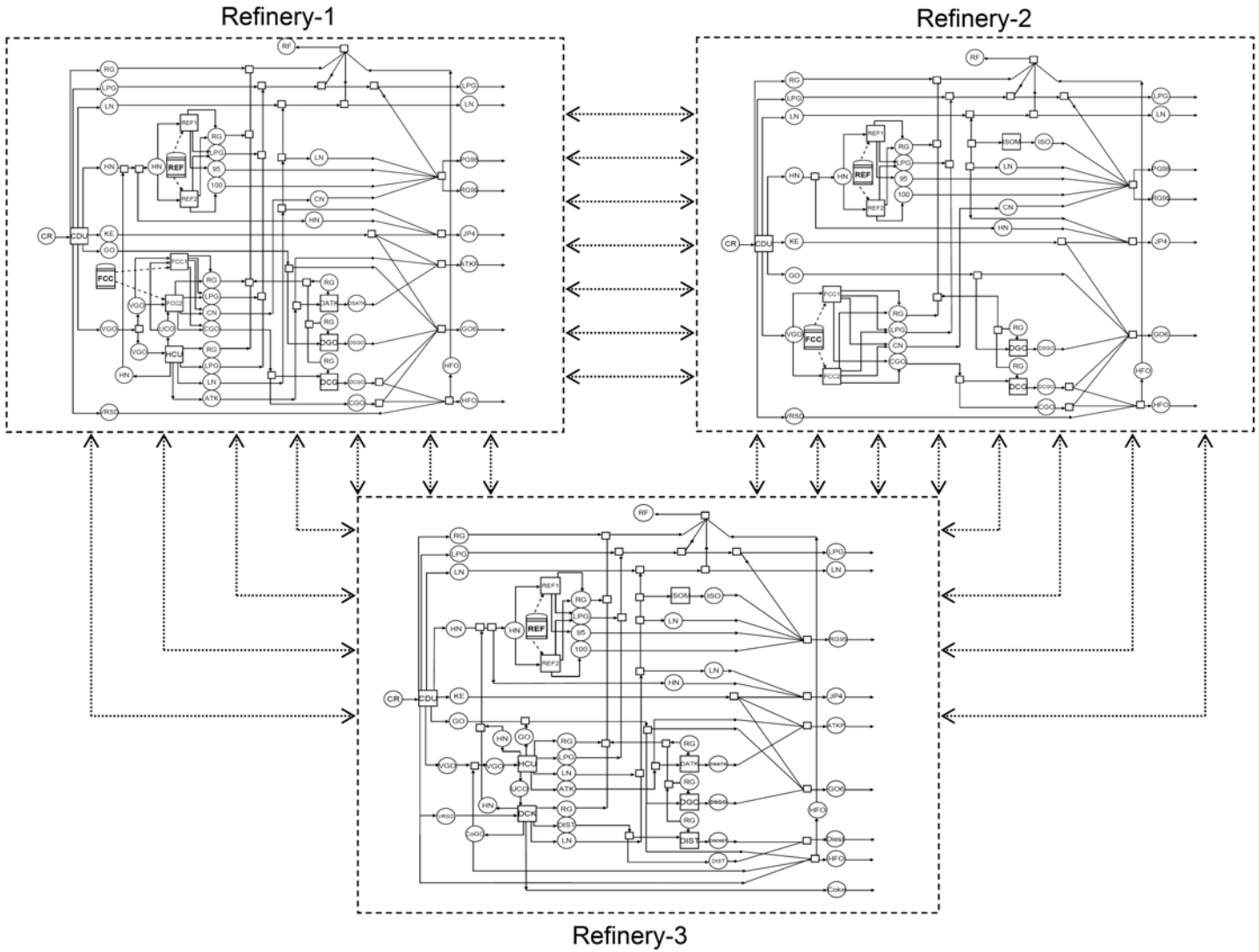

Figure 7.2 SEN representation of the refinery integration network.

Table 7.2 Major products and process technologies in the petrochemical complex

Product	Sale Price ($/ton)*	Process Technology	Process Index	Min Econ. Prod. (10^3 ton/yr)
Ethylene (E)	1570	Pyrolysis of naphtha (low severity)	1	250
		Pyrolysis of gas oil (low severity)	2	250
		Steam cracking of naphtha (high severity)	3	250
		Steam cracking of gas oil (high severity)	4	250
Ethylene Dichloride (EDC)	378	Chlorination of ethylene	5	180
		Oxychlorination of ethylene	6	180
Vinyl chloride monomer (VCM)	1230	Chlorination and Oxychlorination of ethylene	7	250
		Dehydrochlorination of ethylene dichloride	8	125
Polyvinyl chloride (PVC)	1600	Bulk polymerization	9	50
		Suspension polymerization	10	90

* All chemical prices in this study were obtained from latest CW Price Reports in the chemical week journal.

The modeling system GAMS (Brooke et al., 1996) is used for setting up the optimization models. The computational tests were carried out on a Pentium M processor 2.13 GHz and the MILP problems were solved with CPLEX (CPLEX Optimization Inc, 1993).

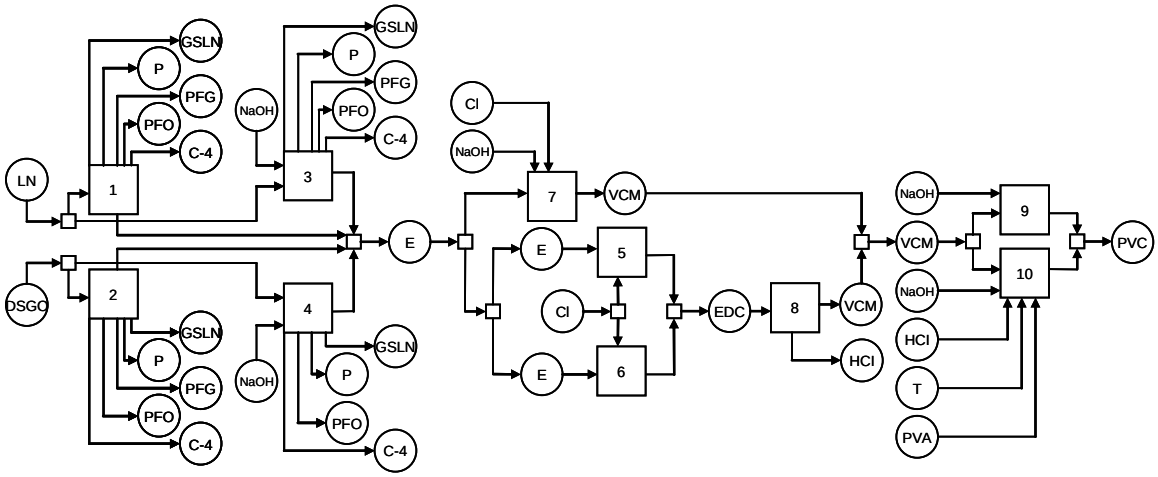

Figure 7.3 SEN representation of the PVC petrochemical complex possible routes.

The problem was first solved for the refinery network separately in order to compare and illustrate the effect of considering the PVC complex on the refinery network design and operating policies. Table 7.3 shows the optimal network integration design and operating policies of the refineries. The three refineries collaborated to satisfy a given local market demand and the model proposed the production and blending level targets for the individual sites. The annual production cost across the facilities was found to be $9,331,000.

Table 7.3 Model results of multirefinery network

Process variables				**Results (10^3 ton/yr)**		
				R1	**R2**	**R3**
Crude oil supply				4500.0	12000.0	9900.0
Production levels	Crude unit			4500.0	12000.0	9900.0
	Reformer			573.1	1824.5	1800.0
	Isomerization			200.0	-	450.0
	FCC			640.0	1400.0	-
	Hydrocracker			-	1740.4	2400
	Delayed coker			-	-	1484
	Des Gas oil			1084.6	2763.7	2383.8
	Des cycle gas oil			200.0	600.0	-
	Des ATK			-	1200.0	1654.8
	Des Distillates			-	-	360
Intermediate streams exchange	**From**	**R1**	VGO	-	-	446.0 to HCU
			VRSD	-	-	380.4 to Coker
		R2	LN	-	-	340.0 to Isomer
		R3	LN	86.1 to Isomer	-	-
			VGO	-	144.7 to FCC	-
			UCO	-	130.1 to FCC	-
Exports	PG95				273.2	
	JP4				1359.5	
	GO6				3695.7	
	HFO				1579.8	
	ATK				1767.5	
	Coke				203.9	
	Diesel				109.7	
Total cost ($/yr)					$9,331,000	

The model was then solved for the total refinery network and the PVC petrochemical complex. As shown in result Table 7.4, the proposed model redesigned the refinery network and operating policies and also devised the optimal production plan for the PVC complex

from all available process technologies. The model selected gas oil, an intermediate refinery stream, as the refinery feedstock to the petrochemical complex as opposed to the normally used light naphtha feedstock in industrial practice. In fact, this selection provided the optimal strategy as the light naphtha stream was used instead in the gasoline pool for maximum gasoline production. PVC production was proposed by first the high severity steam cracking of gas oil to produce ethylene. Vinyl chloride monomer (VCM) is then produced

Table 7.4 Deterministic model results of refinery and petrochemical networks

	Process variables				**Results (10^3 ton/yr)**		
					R1	**R2**	**R3**
Refinery	**Crude oil supply**				4500.0	12000.0	9900.0
	Production levels	Crude unit			4500.0	12000.0	9900.0
		Reformer			573.1	1824.6	1793.5
		Isomerization			200.0	-	450.0
		FCC			640.0	1400.0	-
		Hydrocracker			-	1740.4	2400.0
		Delayed coker			-	-	1440.0
		Des Gas oil			1300.0	3000.0	2400.0
		Des cycle gas oil			200.0	600.0	-
		Des ATK			-	1200.0	1654.8
		Des Distillates			-	-	360.0
	Intermediate streams exchange	**From**	**R1**	VGO	-	204.4 to HCU	301.2 to HCU
			R2	LN	-	-	321.2 to Isom
				VRSD	-	-	267.6 to Coker
			R3	LN	68.0 to Isom		
				UCO	-	100.3 to FCC	-
	Exports	PG95				265.2	
		JP4				1365.5	
		GO6				1503.4	
		HFO				1658.9	
		ATK				1767.5	
		Coke				178.8	
		Diesel				84.0	
Petrochemical	**Refinery feed to PVC complex**	Gas oil			1162.4	920.0	71.3
	Production levels	S. Crack GO (4)				552.2	
		Cl & OxyCl E (7)				459.1	
		Bulk polym. (9)				204.0	
	Final Products	PVC				204.0	
Total cost ($/yr)						$8,948,000	

through the chlorination and oxychlorination of ethylene and finally, VCM is converted to PVC by bulk polymerization. The simultaneous optimization of the refinery and petrochemical network had an impact on both the refinery intermediate exchange network and production levels, as shown in Tables 7.3 and 7.4. For example, the capacity utilization of the desulfurization of gas oil process increased from 83%, 92%, 99% in refineries 1, 2, and 3, respectively, to 100% in all refineries when the petrochemical network was considered in the model. The annual production cost across the facilities was found to be $8,948,000.

7.5 Conclusion

A mixed-integer programming model for designing an integration and coordination policy among multiple refineries and a petrochemical network was presented. The objective was to develop a simultaneous methodology for designing a process integration network between petroleum refining and the petrochemical industry. A large-scale three refinery network and a PVC petrochemical complex were integrated to illustrate the performance of the proposed design methodology and to show the economic potential and trade-offs involved in the optimization of such systems. The study showed that the optimization of the downstream petrochemical industry has an impact on the multirefinery network integration and coordination strategies. This result emphasizes the importance of developed methodology.

In our study, however, all parameters were assumed to be known with certainty. Nevertheless, the current situation of fluctuating and high petroleum crude oil prices, changes in demand, and the direct effect this can have on the downstream petrochemical system underlines the importance of considering uncertainties. For example, the availability of

crude oils, feedstock and chemicals prices, and market demands for finished products will have a direct impact on the output of the highly strategic decisions involved in our study. Acknowledging the shortcomings of deterministic models, the next phase of our investigation will be the consideration of uncertainties in the integration problem.

Chapter 8

Integration and Coordination of Multisite Refinery and Petrochemical Networks under Uncertainty

8.1 Introduction

In this final chapter, we study the multisite refinery and petrochemical integration problem, explained in Chapter 7, under uncertainty. The randomness considered includes both the objective function and right-hand side parameters of inequality constraints. As pointed out in the previous chapters, considering such strategic planning decisions requires proper handling of uncertainties as they play a major role in the final decision making.

The main focus of this study is to develop a mathematical programming tool for simultaneous design of an integrated network of refineries and petrochemical processes under uncertainty. The proposed model not only addresses the integration between the multiple refineries and devises their detailed plans, but also establishes the design of an optimal petrochemical network from a range of process technologies to satisfy a given demand. In this study we treat parameter uncertainty in terms of imported crude oil price, refinery product price, petrochemical product price, refinery market demand, and petrochemical lower level product demand. The problem is modeled as an MILP two-stage stochastic model with recourse. Furthermore, we apply the sample average approximation (SAA) method within an iterative scheme to generate the required scenarios. The solution

quality is then statistically evaluated by measuring the optimality gap of the final solution. The objective function is a minimization of the annualized cost over a given time horizon among the refineries by improving the coordination and utilization of excess capacities in each facility and maximization of the added value in the petrochemical system. The proposed formulation was applied to an integrated industrial scale case study of a petrochemical complex for the production of polyvinyl chloride (PVC) and a network of petroleum refineries.

The remainder of Chapter 8 is organized as follows. In the following section we will explain the proposed model formulation for the refinery and petrochemical integration problem under uncertainty. Then we will explain the scenario generation methodology adopted, in section 8.3. In section 8.4, we present the computational results and the performance of the proposed approach on an industrial scale case study. The chapter ends with concluding remarks in section 8.5.

8.2 Model Formulation

The proposed formulation addresses the problem of planning an integrated network of refineries and petrochemical processes. The proposed model is based on the formulation proposed in the previous chapters of this thesis. The general problem under study was defined in the previous chapter. In this study, uncertainty was accounted for by using two-stage stochastic programming with recourse approach. Parameters uncertainties considered in this study included uncertainties in the imported crude oil price $CrCost_{cr}$, refinery product price Pr_{cfr}^{Ref}, petrochemical product price Pr_{cp}^{Pet}, refinery market demand $D_{Ref_{cfr}}$, and

petrochemical lower level product demand $D_{Pet}{}^{L}_{cp}$. Uncertainty is modeled through the use of mutually exclusive scenarios of the model parameters with a finite number N of outcomes. For each $\xi_k = (CrCost_{cr,k},\ Pr^{Ref}_{cfr,k},\ Pr^{Pet}_{cp,k},\ D_{Ref_{cfr,k}},\ D_{Pet}{}^{L}_{cp,k})$ where $k = 1,2,...,N$, there corresponds a probability p_k. The generation of the scenarios will be explained in a later section. The proposed stochastic model is as follows:

$$
\begin{aligned}
Min \quad & \sum_{cr\in CR}\sum_{i\in I}\sum_{k\in N} p_k\, CrCost_{cr,k}\, S^{Ref}_{cr,i} + \sum_{p\in P} OpCost_p \sum_{cr\in CR}\sum_{i\in I} z_{cr,p,i} \\
& + \sum_{cir\in CIR}\sum_{i\in I}\sum_{i'\in I} InCost_{i,i'}\, ypipe^{Ref}_{cir,i,i'} + \sum_{i\in I}\sum_{m\in M_{Ref}}\sum_{s\in S} InCost_{m,s}\, yexp^{Ref}_{m,i,s} \\
& - \sum_{cfr\in PEX}\sum_{i\in I}\sum_{k\in N} p_k\, Pr^{Ref}_{cfr,k}\, e^{Ref}_{cfr,i} - \sum_{cp\in CP}\sum_{m\in M_{Pet}}\sum_{k\in N} p_k\, Pr^{Pet}_{cp,k}\, \delta_{cp,m}\, x^{Pet}_{m} \qquad \text{where } i \neq i' \\
& + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref+}_{cfr}\, V^{Ref+}_{cfr,k} + \sum_{cfr\in CFR}\sum_{k\in N} p_k\, C^{Ref-}_{cfr}\, V^{Ref-}_{cfr,k} \\
& + \sum_{cp\in CFP}\sum_{k\in N} p_k\, C^{Pet+}_{cp}\, V^{Pet+}_{cp,k} + \sum_{cp\in CFP}\sum_{k\in N} p_k\, C^{Pet-}_{cp}\, V^{Pet-}_{cp,k}
\end{aligned}
\tag{8.1}
$$

Subject to

$$
z_{cr,p,i} = S^{Ref}_{cr,i} \qquad \forall\ cr \in CR,\ i \in I \quad \text{where } p \in P' = \{\text{Set of CDU processes } \forall \text{ plant i}\} \tag{8.2}
$$

$$
\begin{aligned}
& \sum_{p\in P} \alpha_{cr,cir,i,p}\, z_{cr,p,i} + \sum_{i'\in I}\sum_{p\in P} \xi_{cr,cir,i',p,i}\, xi^{Ref}_{cr,cir,i',p,i} - Fi^{Pet}_{cr,cir\in RPI,i} \\
& - \sum_{i'\in I}\sum_{p\in P} \xi_{cr,cir,i,p,i'}\, xi^{Ref}_{cr,cir,i,p,i'} - \sum_{cfr\in CFR} w_{cr,cir,cfr,i} - \sum_{rf\in FUEL} w_{cr,cir,rf,i} = 0
\end{aligned}
\qquad
\begin{aligned}
& \forall\ cr\in CR,\ cir\in CIR,\ i'\ \&\ i\in I \\
& \text{where } i \neq i'
\end{aligned}
\tag{8.3}
$$

$$
\sum_{cr\in CR}\sum_{cir\in CB} w_{cr,cir,cfr,i} - \sum_{cr\in CR}\sum_{rf\in FUEL} w_{cr,cfr,rf,i} - \sum_{cr\in CR} Ff^{Pet}_{cr,cfr\in RPF,i} = x^{Ref}_{cfr,i} \qquad \forall\ cfr \in CFR,\ i \in I \tag{8.4}
$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\frac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} = xv^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ i\in I \qquad (8.5)$$

$$\sum_{cir\in FUEL} cv_{rf,cir,i}\ w_{cr,cir,rf,i} + \sum_{cfr\in FUEL} w_{cr,cfr,rf,i} - \sum_{p\in P}\beta_{cr,rf,i,p}\ z_{cr,p,i} = 0 \qquad \forall\ cr\in CR,\ rf\in FUEL,\ i\in I \qquad (8.6)$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\left(\begin{array}{l} att_{cr,cir,q\in Qv}\ \dfrac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} + att_{cr,cir,q\in Qw} \\ \left[w_{cr,cir,cfr,i} - \sum_{rf\in FUEL} w_{cr,cfr,rf,i} - \sum_{cr\in CR} Ff^{Pet}_{cr,cfr\in RPF,i} \right] \end{array}\right) \geq q^{L}_{cfr,q\in Qv}\ xv^{Ref}_{cfr,i} + q^{L}_{cfr,q\in Qw}\ x^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ q=\{Qw,Qv\},\ i\in I \qquad (8.7)$$

$$\sum_{cr\in CR}\sum_{cir\in CB}\left(\begin{array}{l} att_{cr,cir,q\in Qv}\ \dfrac{w_{cr,cir,cfr,i}}{sg_{cr,cir}} + att_{cr,cir,q\in Qw} \\ \left[w_{cr,cir,cfr,i} - \sum_{rf\in FUEL} w_{cr,cfr,rf,i} - \sum_{cr\in CR} Ff^{Pet}_{cr,cfr\in RPF,i} \right] \end{array}\right) \leq q^{U}_{cfr,q\in Qv}\ xv^{Ref}_{cfr,i} + q^{U}_{cfr,q\in Qw}\ x^{Ref}_{cfr,i} \qquad \forall\ cfr\in CFR,\ q=\{Qw,Qv\},\ i\in I \qquad (8.8)$$

$$MinC_{m,i} \leq \sum_{p\in P}\gamma_{m,p}\sum_{cr\in CR} z_{cr,p,i} \leq MaxC_{m,i} + \sum_{s\in S} AddC_{m,i,s}\ yexp^{Ref}_{m,i,s} \qquad \forall\ m\in M_{Ref}, i\in I \qquad (8.9)$$

$$\sum_{cr\in CR}\sum_{p\in P}\xi_{cr,cir,i,p,i'}\ xi^{Ref}_{cr,cir,i,p,i'} \leq F^{U}_{cir,i,i'}\ ypipe^{Ref}_{cir,i,i'} \qquad \forall\ cir\in CIR,\ i'\ \&\ i\in I \text{ where } i\neq i' \qquad (8.10)$$

$$\sum_{i\in I}\left(x^{Ref}_{cfr,i} - e^{Ref}_{cfr',i}\right) + V^{Ref+}_{cfr,k} - V^{Ref-}_{cfr,k} = D_{Ref_{cfr,k}} \qquad \forall\ cfr\in CFR,\ cfr'\in PEX,\ k\in N \qquad (8.11)$$

$$IM_{cr}^{L} \le \sum_{i \in I} S_{cr,i}^{Ref} \le IM_{cr}^{U} \qquad \forall \ cr \in CR \tag{8.12}$$

$$Fn_{cp \in NRF}^{Pet} + \sum_{i \in I} \sum_{cr \in CR} Fi_{cr,cp \in RPI,i}^{Pet} + \sum_{i \in I} \sum_{cr \in CR} Ff_{cr,cp \in RPF,i}^{Pet} + \sum_{m \in M_{Pet}} \delta_{cp,m} \ x_m^{Pet} + V_{cp \in CFP,k}^{Pet+} - V_{cp \in CFP,k}^{Pet-} = D_{Pet}{}_{cp \in CFP,k}^{L} + xi_{cp \in CIP}^{Pet} \qquad \forall \ \begin{matrix} cp \in CP \\ k \in N \end{matrix} \tag{8.13}$$

$$Fn_{cp \in NRF}^{Pet} + \sum_{i \in I} \sum_{cr \in CR} Fi_{cr,cp \in RPI,i}^{Pet} + \sum_{i \in I} \sum_{cr \in CR} Ff_{cr,cp \in RPF,i}^{Pet} + \sum_{m \in M_{Pet}} \delta_{cp,m} \ x_m^{Pet} \le D_{Pet}{}_{cp \in CFP}^{U} \qquad \forall \ cp \in CP \tag{8.14}$$

$$B_m^{L} \ y_{proc}{}_m^{Pet} \le x_m^{Pet} \le K^{U} \ y_{proc}{}_m^{Pet} \qquad \forall \ m \in M_{Pet} \tag{8.15}$$

$$\sum_{cp \in CIP} y_{proc}{}_m^{Pet} \le 1 \qquad \forall \ m \in M_{Pet} \text{ that produces } cp \in CIP \tag{8.16}$$

$$\sum_{cp \in CFP} y_{proc}{}_m^{Pet} \le 1 \qquad \forall \ m \in M_{Pet} \text{ that produces } cp \in CFP \tag{8.17}$$

$$Fn_{cp}^{Pet} \le S_{cp}^{Pet} \qquad \forall \ cp \in NRF \tag{8.18}$$

The above formulation is an extension of the deterministic model explained in the previous chapter. We will mainly explain the stochastic part of the above formulation. The above formulation is a two-stage stochastic mixed-integer linear programming (MILP) model. Objective function (8.1) minimizes the first stage variables and the penalized second stage variables. The production over the target demand is penalized as an additional inventory cost per ton of refinery and petrochemical products. Similarly, shortfall in a certain product demand is assumed to be satisfied at the product spot market price. The

recourse variables $V_{cfr,k}^{Ref+}$, $V_{cfr,k}^{Ref-}$, $V_{cp,k}^{Pet+}$ and $V_{cp,k}^{Pet-}$ in equations (8.11) and (8.13) represent the refinery production shortfall and surplus as well as the petrochemical production shortfall and surplus, respectively, for each random realization $k \in N$. These variables will compensate for the violations in equations (8.11) and (8.13) and will be penalized in the objective function using appropriate shortfall and surplus costs C_{cfr}^{Ref+} and C_{cfr}^{Ref-} for the refinery products, and C_{cp}^{Pet+} and C_{cp}^{Pet-} for the petrochemical products, respectively. Uncertain parameters are assumed to follow a normal distribution for each outcome of the random realization ξ_k. Although this might sound restrictive, this assumption imposes no limitation on the generality of the proposed approach as other distributions can be easily incorporated instead. Furthermore, in equation (8.13) an additional term xi_{cp}^{Pet} was added to the left hand side representing the flow of intermediate petrochemical stream of $cp \in CIP$. This term may be set to zero under the assumption that intermediate petrochemical streams produced by any process are consumed within the petrochemical network. However, this assumption may not be valid when considering a subsystem of the petrochemical network.

8.3 Scenario Generation

The solution of stochastic problems is generally very challenging as it involves numerical integration over the random continuous probability space of the second stage variables (Goyal and Ierapetritou, 2007). An alternative approach is the discretization of the random space using a finite number of scenarios. A common approach is the Monte Carlo sampling where independent pseudo-random samples are generated and assigned equal probabilities (Ruszczyński and Shapiro, 2003). In our study, the Sample Average Approximation (SAA)

method, also known as stochastic counterpart, is employed. The SAA problem can be written as (Verweij et al. 2003):

$$v_N = \min_{x \in X} c^T x + \frac{1}{N} \sum_{k \in N} Q(x, \xi^k) \tag{8.19}$$

It approximates the expectation of the stochastic formulation (usually called the "true" problem) and can be solved using deterministic algorithms. Problem (8.19) can be solved iteratively in order to provide statistical bounds on the optimality gap of the objective function value. The iterative SAA procedure steps are explained in section 4.4 of Chapter 4.

8.4 Illustrative Case Study

This section presents the computational results of the proposed model and sampling scheme. We examine the same case study considered in Chapter 7 of the three refineries and the PVC complex. In this study, we considered uncertainty in the imported crude oil price, refinery product price, petrochemical product price, refinery market demand, and petrochemical lower level product demand. The major capacity constraints for the refinery network are given in Table 8.1 and the process technologies considered for the production of PVC are listed in Table 8.2. The representation for the topology of the refineries network and petrochemical technologies for the PVC production are given in Figure 7.2 and Figure 7.3, respectively, in Chapter 7. In the presentation of the results, we focus on demonstrating the sample average approximation computational results as we vary the sample sizes and compare their solution accuracy and the CPU time required for solving the models.

Table 8.1 Major refinery network capacity constraints

Production Capacity	**Higher limit (10^3 ton/yr)**		
	R1	R2	R3
Distillation	45000.	12000.0	9900.0
Reforming	700.0	2000.0	1800.0
Isomerization	200.0	-	450.0
Fluid catalytic cracker	800.0	1400.0	-
Hydrocracker	-	1800.0	2400.0
Delayed coker	-	-	1800
Des gas oil	1300.0	3000.0	2400.0
Des cycle gas oil	200.0	750.0	-
Des ATK	-	1200.0	1680.0
Des Distillates	-	-	450.0
Crude availability			
Arabian Light		31200.0	
Local Demand			
LPG		$\mathcal{N}(432,20)$	
LN		-	
PG98		$\mathcal{N}(400,20)$	
PG95		$\mathcal{N}(4390,50)$	
JP4		$\mathcal{N}(2240,50)$	
GO6		$\mathcal{N}(4920,50)$	
ATK		$\mathcal{N}(1700,50)$	
HFO		$\mathcal{N}(200,20)$	
Diesel		$\mathcal{N}(400,20)$	
Coke		$\mathcal{N}(300,20)$	

The modeling system GAMS (Brooke et al., 1996) is used for setting up the optimization models. The computational tests were carried out on a Pentium M processor 2.13 GHz and the MILP problems were solved with CPLEX (CPLEX Optimization Inc, 1993).

The problem was solved for different sample sizes N and N' to illustrate the variation of optimality gap confidence intervals, while fixing the number of replications R to 30. The replication number R need not be very large to get an insight of $\bar{v}_N$ variability. Table 8.3 shows different confidence interval values of the optimality gap when the sample size of N assumes values of 1000, 2000, and 3000 while varying N' from 5000, 10000, to 20000 samples. The sample sizes N and N' were limited to these values due to increasing

computational effort. In our case study, we ran into memory limitations when N and N' values exceeded 3000 and 20000, respectively. The solution of the three refineries network and the PVC complex using the SAA scheme with $N = 3000$ and $N' = 20000$ required 1114 CPU sec to converge to the optimal solution.

Table 8.2 Major products and process technologies in the petrochemical complex

Product	Sale Price ($/ton)	Process Technology	Process Index	Min Econ. Prod. (10^3 ton/yr)
Ethylene (E)	$\mathcal{N}(1570,10)$	Pyrolysis of naphtha (low severity)	1	250
		Pyrolysis of gas oil (low severity)	2	250
		Steam cracking of naphtha (high severity)	3	250
		Steam cracking of gas oil (high severity)	4	250
Ethylene Dichloride (EDC)	$\mathcal{N}(378,10)$	Chlorination of ethylene	5	180
		Oxychlorination of ethylene	6	180
Vinyl chloride monomer (VCM)	$\mathcal{N}(1230,10)$	Chlorination and Oxychlorination of ethylene	7	250
		Dehydrochlorination of ethylene dichloride	8	125
Polyvinyl chloride (PVC)	$\mathcal{N}(1600,10)$	Bulk polymerization	9	50
		Suspension polymerization	10	90

Table 8.4 depicts the results of the optimal integration network between the three refineries and the PVC petrochemical complex. As shown in Table 8.4, the proposed model redesigned the refinery integration network topology and operating policies when compared to the deterministic solution obtained in Chapter 7. However, similar to the deterministic solution the model selected gas oil, an intermediate refinery stream, as the refinery feedstock to the petrochemical complex as opposed to typically used light naphtha feedstock. This selection emphasizes the importance of sparing the light naphtha stream for the gasoline pool to get maximum gasoline production.

Table 8.3 Computational results with SAA for the stochastic model

		Lower bound sample size=N		
		1000	2000	3000
UB Sample Size	Number of Samples: R=30			
N'=5000	LB estimate: $\overline{v}_N$	8802837	8804092	8804456
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	3420	2423	1813
	UB estimate: $\hat{v}_{N'}$	8805915	8805279	8805578
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	7776	7715	7778
	95% Conf. Interval	[0,14274]	[0,11324]	[0,10713]
	CPU (sec)	65	112	146
N'=10000	LB estimate: $\overline{v}_N$	8800071	8802080	8804305
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	3356	2527	2010
	UB estimate: $\hat{v}_{N'}$	8803310	8803204	8803414
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	5473	5833	5410
	95% Conf. Interval	[0,12068]	[0,9484]	[0,7420]
	CPU (sec)	196	224	263
N'=20000	LB estimate: $\overline{v}_N$	8796058	8801812	8802511
	LB error: $\widetilde{\varepsilon}_l$ (α=0.975)	3092	2345	1755
	UB estimate: $\hat{v}_{N'}$	8802099	8804121	8802032
	UB error: $\widetilde{\varepsilon}_u$ (α=0.975)	3837	3886	3880
	95% Conf. Interval	[0,12970]	[0,8540]	[0,5635]
	CPU (sec)	1058	1070	1114

PVC production, on the other hand, is carried out by first high severity steam cracking of gas oil to produce ethylene. Vinyl chloride monomer (VCM) is then produced through the chlorination and oxychlorination of ethylene and finally, VCM is converted to PVC by bulk polymerization. The annual production cost across the refineries and the PVC complex was $8,802,000.

Table 8.4 Stochastic model results of refinery and petrochemical networks

Process variables				Results (10^3 ton/yr)		
				R1	**R2**	**R3**
Refinery	**Crude oil supply**			4500.0	12000.0	9900.0
	Production levels	Crude unit		4500	12000	9900
		Reformer		612.5	1824.6	1784.6
		Isomerization		160	-	450
		FCC		378	1174.2	-
		Hydrocracker		-	1740.4	2400
		Delayed coker		-	-	1440
		Des Gas oil		1300	3000	2400
		Des cycle gas oil		168.6	600	-
		Des ATK		-	1200	1654.8
		Des Distillates		-	-	366.2
	Intermediate streams exchange	**From**	**R1** VGO	-	-	576.1 to HCU
			R2 LN	-	-	112.4 to Isom
			R3 VGO	-	274.8 to FCC	-
	Exports	PG95			439.8	
		JP4			1101.9	
		GO6			2044.2	
		HFO			1907.8	
		ATK			1887.6	
		Coke			110.7	
		Diesel			5.1	
Petrochemical	**Refinery feed to PVC complex**	Gas oil		788.6	1037.0	71.3
	Production levels	S. Crack GO (4)			486.8	
		Cl & OxyCl E (7)			475.4	
		Bulk polym. (9)			220.0	
	Final Products	PVC			220.0	
Total cost ($/yr)					$8,802,000	

8.5 Conclusion

In this chapter, we proposed a two-stage stochastic mixed-integer programming model for designing an integration and coordination policy among multiple refineries and a petrochemical network under uncertainty. Uncertainty was considered in the parameters of imported crude oil price, refinery product price, petrochemical product price, refinery market demand, and petrochemical lower level product demand. The approach employs the sample average approximation (SAA) method with a statistical bounding and validation technique.

In this sampling scheme, a relatively small sample size N is used to make decisions, with multiple replications, and another independent larger sample is used to reassess the objective function value while fixing the first stage variables. The proposed model performance was illustrated on a network of three large-scale refineries and a PVC petrochemical complex. The formulation captured the simultaneous design of both the refinery and petrochemical networks and illustrated the economic potential and trade-offs. The consideration of uncertainties in this type of high level strategic planning model, especially with the current volatile market environment, presented an adequate treatment of the problem and a proper optimization tool.

Chapter 9

Conclusion

In this chapter we highlight the key contributions of this dissertation and provide some recommendations for possible research extensions.

9.1 Key Contributions

Multisite Refinery Planning

- Developed a framework for the design and analysis of multisite integration and coordination strategies within a network of petroleum refineries through a mixed-integer linear programming (MILP) technique.

- Extended the proposed model to account for model uncertainty by means of two-stage stochastic programming. Parameters uncertainty considered include coefficients of the objective function and right-hand-side parameters in the inequality constraints.

- The proposed stochastic model makes use of the sample average approximation (SAA) method with statistical bounding techniques to give an insight on the sample size required to give adequate approximation of the problem.

- Applied a robust optimization technique to investigate both model robustness and solution robustness, where each measure is assigned a scaling factor to analyze the sensitivity of the refinery plan and integration network due to variations.

Petrochemical Industry Planning

- Proposed a two-stage stochastic programming model to address the strategic planning, design and optimization of a network of petrochemical processes under uncertainty. Parameter uncertainty considered in this part includes process yield, raw material and product prices, and lower product market demand.

- The Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) were investigated to numerically illustrate the value of including the randomness of the different model parameters.

- Applied a robust optimization technique to investigate both model robustness and solution robustness, where each measure is assigned a scaling factor to analyze the sensitivity of the petrochemical network.

Integration and Coordination of Multisite Refinery and Petrochemical Networks

- Proposed a formulation that addresses the design of optimal integration and coordination strategy of multisite refinery and petrochemical networks. The proposed model provided a proper planning tool for the petroleum refining and petrochemical industry. The

optimal production strategy was achieved by allowing trade offs between the refinery and the downstream petrochemical markets.

- Extended the proposed model in this dissertation to account for various parameter uncertainties using two-stage stochastic programming.

- The proposed approach uses the sample average approximation (SAA) method with statistical bounding techniques to give an insight on the sample size requirement and optimality gap estimation.

9.2 Future Research

The following recommendations emerged as a result of the work presented and the objectives pursued in this thesis. Future work on these recommendations can extend and improve the work developed in this dissertation.

Multisite Refinery Planning

- The integrated network design presented in this thesis specifically addresses intermediate material transfer between processing units at each site. However, utilities integration of all forms including fuel oil, fuel gas, hydrogen, electrical power, and steam, is of great importance. As discussed in Chapter 2, the benefits of including the utilities in the integration problem can yield significant energy savings. More work is needed to properly capture such benefits.

- The objective function considered in this dissertation merely considered economics in terms of cost and profit. However, with the increasingly strict regulations on

environmental standards, emission control on various pollutants and green house gases should be considered. Future work in this area should take into account different mitigation alternatives for dealing with such emission sources in the refinery.

- The framework presented assumes the prior knowledge of the available sets of states, tasks, and requirement. However, defining these sets based on the available supply, demand and market prices remains a problem that requires further investigation.

Petrochemical Industry Planning

- The model proposed in this dissertation presented the overall optimal network of the petrochemical processes based on the available supply demand market prices. The implementation of such highly capital intensive projects would normally be phased based on the market demand shifts and budget constraints. In order to properly address these issues, a multiperiod optimization model is required in addition to considering uncertainty in each forecasted period. Further research towards this objective needs to be developed.

- Similar to the point mentioned earlier, future research needs to account for environmental regulations and the selection of emissions control alternatives.

Integration and Coordination of Multisite Refinery and Petrochemical Networks

- In this dissertation we merely considered the uncertainty in the model parameters without including robustness measures. This is due to the fact that modeling robustness using

variance as shown in the multisite refinery and petrochemical systems renders the problem nonlinear. Solving such large scale MINLP models might lead to complications that can be avoided if a different measure is used to capture the risk notion in the problem. More recently introduced financial risk measures, including the Value-at-Risk (VaR) and Conditional Value-at-Risk (CVaR), should be pursued.

Appendix

SAA Optimal Solution Bounding

Here we present a proof of the SAA lower bound on the true optimal solution of the stochastic problem. The proof is rather intuitive, but for more details we refer the reader to Mark et al. (1999).

Proposition 1. For any R independent and identically distributed sample batches (denoting the number of sample replication) each with sample size of N, i.e. $\xi^{j1},...,\xi^{jN}$, $j = 1,...,R$, the $\mathrm{E}[\nu_N^j] \le \nu^*$ is always valid.

Proof.

For any feasible point x' that belongs to the solution set X, the inequality below is valid:

$$\hat{f}_N(x') \ge \min_{x \in X} \hat{f}_N(x)$$

By taking the expectations of both sides and minimizing the left hand side, we get:

$$\min_{x \in X} \mathrm{E}[\hat{f}_N(x)] \ge \mathrm{E}[\min_{x \in X} \hat{f}_N(x)]$$

Since $\mathrm{E}[\hat{f}_N(x)] = f(x)$, it follows that $\nu^* \ge \mathrm{E}[\nu_N^j]$. □

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Publication

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