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*Khalid Y. Al-Qahtani and Ali Elkamel*

# **Planning and Integration of Refinery and Petrochemical Operations**



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## Preface

Petroleum refining and the petrochemical industry account for a major share of the world energy and industrial market. In many situations, they represent the economic 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. Previous attempts in the field either studied the two systems in isolation or assumed limited interactions between them.

This book aims at providing the reader with a detailed understanding of the planning, integration and coordination of multisite refinery and petrochemical networks using proper deterministic and stochastic techniques. The book consists of three parts:

- **Part 1:** Background
- **Part 2:** Deterministic Planning Models
- **Part 3:** Planning under Uncertainty

Part 1, comprised of one chapter, introduces the reader to the configuration of petroleum refining and the petrochemical industry. It also discusses key classifications of petrochemical industry feedstock from petroleum products. The final part explains and proposes possible synergies between the petroleum refinery and the petrochemical industry.

Part 2, comprised of four chapters, focusses on the area of planning in petroleum refining and the petrochemical industry under deterministic conditions. Chapter 2 discusses the model classes used in process planning (i.e., empirical models, and first principle models) and provides a series of case studies to illustrate the concepts and impeding assumptions of the different modeling approaches. Chapter 3 tackles the integration and coordination of a multisite refinery network. It addresses the design and analysis of multisite integration and coordination strategies within a network of petroleum refineries through a mixed-integer linear programming (MILP) technique. Chapter 4 explains the general representation of a petrochemical planning model which selects the optimal network from the overall petrochemical superstructure. The system is modeled as a MILP problem and is illustrated via a

numerical example. Chapter 5 addresses the integration between the multisite refinery system and the petrochemical industry. The chapter develops 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 proposed approach is the development of a methodology for the simultaneous analysis of process network integration within a multisite refinery and petrochemical system. Part 2 of this book serves as a foundation for the reader of Part 3.

Part 3, comprised of four chapters, tackles the area of planning in the petroleum refinery and the petrochemical industry under uncertainty. Chapter 6 explains the use of two-stage stochastic programming and the incorporation of risk management for a single site refinery plant. The example used in this chapter is simple enough for the reader to grasp the concept of two-stage stochastic programming and risk management and to be prepared for the larger scale systems in the remaining chapters. Chapter 7 extends the proposed model in Chapter 3 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. Chapter 8 addresses the planning, design and optimization of a network of petrochemical processes under uncertainty and robust considerations. Similar to the previous chapter, 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 the value of the stochastic solution (VSS) are also investigated to illustrate numerically the value of including the randomness of the different model parameters. Chapter 9 extends the petroleum refinery and petrochemical industry integration problem, explained in Chapter 5, 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. The sample average approximation (SAA) method is within an iterative scheme to generate the required scenarios and provide solution quality by measuring the optimality gap of the final solution.

All chapters are equipped with clear figures and tables to help the reader understand the included topics. Furthermore, several appendices are included to explain the general background in the area of stochastic programming, chance constraint programming and robust optimization.

**Part One**  
**Background**



# 1

## Petroleum Refining and Petrochemical Industry Overview

Petroleum refining and the petrochemical industry account for a major share in the world energy and industrial market. In many situations, they represent the economic 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.

In this chapter, we will give an overview of the process configurations of petroleum refining and the petrochemical industry. We will also discuss the key classifications of petrochemical industry feedstock from petroleum products and explain and propose possible synergies between the petroleum refinery and the petrochemical industry.

### 1.1

#### Refinery 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 oil from other crude fractions. During the early years, refining separation was performed using batch processing. However, with the increase in demand for petroleum products, continuous refining became a necessity. The first widely recognized continuous refinery plants emerged around 1912 (Nelson, 1958). With the diversity and complexity of the demand for petroleum products, the refining industry has developed from a few simple processing units to very complex production systems. A simplified process flow diagram of a typical modern refinery is shown in Figure 1.1. For a detailed history of the evolution of refining technologies, we refer the reader to Nelson (1958) and Wilson (1997).

Typically, a refinery is made up of several distinct components that constitute a total production system, as shown in Figure 1.2. These components include:



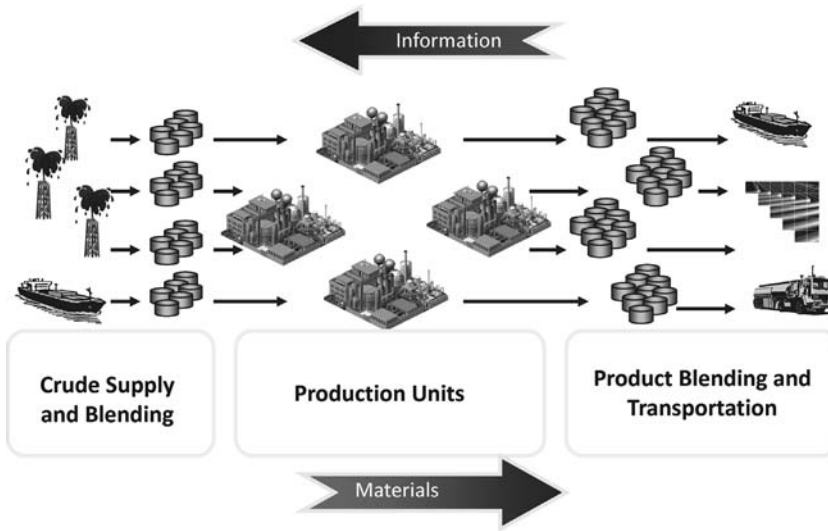


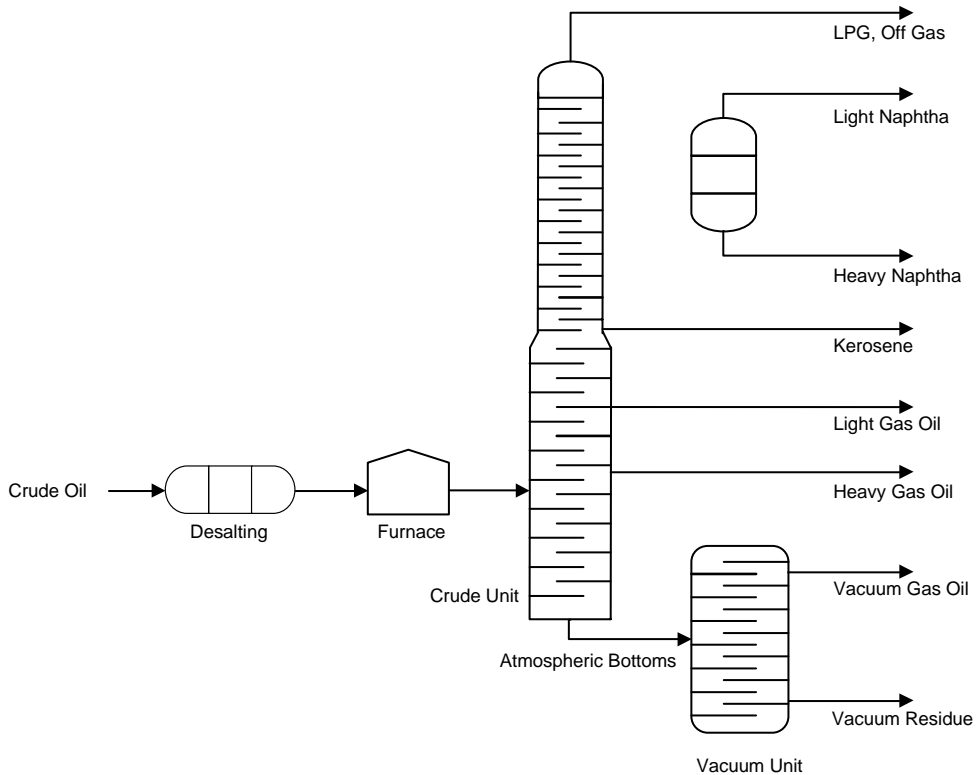
Figure 1.2 Schematic diagram of standard refinery configuration.

- **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. This area also includes the utilities which provide the refinery with fuel, flaring capability, electricity, steam, cooling water, fire water, sweet water, compressed air, nitrogen, and so on, all of which are necessary for the safe operation of the refinery.
- **Product Blending and Transportation:** In this area the final products are processed according to either predetermined recipes and/or to certain product specifications. This area also includes the dispatch (terminals) of finished products to the different customers.

## 1.2

### Mathematical Programming in Refining

The petroleum industry has long made 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 widespread use of linear programming (LP) applications in the industry (Bodington and Baker, 1990). Since then, many early applications followed in the area of refinery planning (Symonds, 1955; Manne, 1958; Charnes and Cooper, 1961; Wagner, 1969; Addams and Griffin, 1972) and distribution planning (Zierer, Mitchell and White, 1976).



**Figure 1.3** Process flow diagram of crude oil distillation process.

One of the main challenges that inspired more research in the area of refining was the blending or pooling problem (Bodington and 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 and 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 and 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 proprietorially developed by refining companies for their own use.

Successive linear programming, 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 the 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 and Waren, 1980). Most commercial blending softwares and computational tools nowadays are based on SLP, such as RPMS by Honeywell Process Solutions (previously Booner and 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.

## 1.3

### Refinery Configuration

#### 1.3.1

##### Distillation Processes

Crude oil distillation is the heart of and major unit in the refinery. Distillation is used to separate oil into fractions by distillation according to their boiling points. Prior to distillation, crude oil is first treated to remove salt content, if higher than 10 lb/1000 bbl, using single or multiple desalting units. This is required in order to minimize corrosion and fouling in the downstream heating trains and distillation columns. As illustrated in Figure 1.3, distillation is usually divided into two steps, atmospheric and vacuum fractionation according to the pressure at which fractionation is achieved. This is done in order to achieve higher separation efficiencies at a lower cost. After heating the crude to near its boiling point, it is introduced to the distillation column in which vapor rising through trays in the column is in direct contact with down-flowing liquid on the trays. During this process, higher boiling point fractions in the vapor phase are condensed and lighter fractions in the liquid are vaporized. This continuous process allows the various fractions of the crude oil with similar boiling points to achieve equilibrium and separate. Liquid can then be drawn off the column at different heights as product and sent for further treating or storage. Common products from the atmospheric distillation column include liquefied petroleum gas (LPG), naphtha, kerosene, gas oils and heavy residues.

The atmospheric bottom, also known as reduced oil, is then sent to the vacuum unit where it is further separated into vacuum gas oil and vacuum residues. Vacuum distillation improves the separation of gas oil distillates from the reduced oil at temperatures less than those at which thermal cracking would normally take place. The basic idea on which vacuum distillation operates is that, at low pressure, the boiling points of any material are reduced, allowing various hydrocarbon components in the reduced crude oil to vaporize or boil at a lower temperature. Vacuum distillation of the heavier product avoids thermal cracking and hence product loss and equipment fouling.

### 1.3.2

#### Coking and Thermal Processes

Nowadays more refineries are seeking lighter and higher quality products out of the heavy residues. Coking and other thermal processes convert heavy feedstocks, usually from distillation processes, to more desirable and valuable products that are suitable feeds for other refinery units. Such units include coking and visbreaking.

One of the widely used coking processes is delayed coking. It involves severe thermal cracking of heavy residues such as vacuum oil, thermal tars, and sand bitumen. The actual coking in this process takes place in the heater effluent surge drum and for this reason the process is called “delayed coking”. The coke produced by this process is usually a hard and porous sponge-like material. This type of coke is called sponge coke and exists in a range of sizes and shapes. Many other types of coke are commercially available in the market and have a wide range of uses, see Table 1.1. Other coking processes, including flexicoking and fluid coking, have been developed by Exxon.

The other thermal cracking process is visbreaking. This is a milder thermal process and is mainly used to reduce the viscosities and pour points of vacuum residues to

**Table 1.1** End use of coke products (Gary and Handwerk, 2001).

| Application   | Coke type | End use                       |
|---------------|-----------|-------------------------------|
| Carbon source | Needle    | Electrodes                    |
|               | Sponge    | Synthetic graphite            |
|               |           | Aluminum anodes               |
|               |           | TiO <sub>2</sub> pigments     |
|               |           | Carbon raiser                 |
|               |           | Silicon carbide               |
|               |           | Foundries                     |
| Fuel use      | Sponge    | Coke ovens                    |
|               |           | Space heating in Europe/Japan |
|               |           | Industrial boilers            |
|               |           | Utilities                     |
|               |           | Cogeneration                  |
|               | Shot      | Lime                          |
|               | Fluid     | Cement                        |
|               | Flexicoke |                               |

meet some types of fuel oil specifications and also to increase catalytic cracker feedstock. The two widely used processes in visbreaking are coil visbreaking and soaker visbreaking. In coil visbreaking most of the cracking takes place in the furnace coil whereas in soaker visbreaking, cracking takes place in a drum downstream of the heater, called the soaker. Each process offers different advantages depending on the given situation.

### 1.3.3

#### **Catalytic Processes**

There are two types of catalytic conversion units in the refinery, cracking and 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 convert 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.

##### **1.3.3.1 Cracking Processes**

Cracking processes mainly include catalytic cracking and hydrocracking. Catalytic cracking involves breaking down and rearranging complex hydrocarbons into lighter molecules in order to increase the quality and quantity of desirable products such as kerosene, gasoline, LPG, heating oil, and petrochemical feedstock. Catalytic cracking follows a similar concept to thermal cracking except that catalysts are used to promote and control the conversion of the heavier molecules into lighter products under much less severe operating conditions. The most commonly used process in the industry is fluid catalytic cracking (FCC) in which oil is cracked in a fluidized catalyst bed where it is continuously circulated between the reaction state and the regeneration state.

Hydrocracking on the other hand is a process that combines catalytic cracking and hydrogenation where the feed is cracked in the presence of hydrogen to produce more desirable products. This process mainly depends on the feedstock characteristics and the relative rates of the two competing reactions, hydrogenation and cracking. In the case where the feedstock has more paraffinic content, hydrogen acts to prevent the formation of polycyclic aromatic compounds. Another important role of hydrogen is to reduce tar formation and prevent buildup of coke on the catalyst.

##### **1.3.3.2 Alteration Processes**

Alteration processes involve rearranging feed stream molecular structure in order to produce higher quality products. One of the main processes in this category is catalytic reforming. Reforming is an important process used to convert low-octane feedstock into high-octane gasoline blending components called reformate. The kinetics of reforming involves a wide range of reactions such as cracking, polymerization, dehydrogenation, and isomerization taking place simultaneously. Depending on the properties of the feedstock, measured by the paraffin, olefin, naphthene,