# 1

# Introduction to Optimization Modeling for Petroleum Refineries

## 1.1 Background

The topological optimization problem for determining an optimal configuration of a petroleum refinery can be addressed by a logic-based modeling approach within a mixed-integer superstructure optimization framework. The focus lies in investigating and advancing existing optimization approaches and strategies of employing logical constraints to conceptual process synthesis and design problems within the framework of conventional mixed-integer linear programming (MILP) (Nemhauser and Wolsey 1988) and alternate generalized disjunctive programming (GDP) (Grossmann and Trespalacios 2013). This work attempts to address the following considerations:

- How the formulation of design specifications in a synthesis problem can be accomplished using logical constraints in a mixed-logical-and-integer optimization model to enrich the problem representation by way of incorporating past design experience, engineering knowledge, and heuristics;
- How structural specifications on the interconnectivity relationships by space (states) and function (tasks) should be properly formulated using logical constraints within a mixed-integer optimization model.

The resulting modeling technique is illustrated on a numerical example, which is based on a case study involving alternative processing routes of naphtha in a refinery.

Process synthesis or conceptual process design is concerned with the identification of the best flowsheet structure to perform a given task. The following variants are mainly available in the literature to address this class of problem: (1) the heuristics method, notably the hierarchical decomposition of design decisions procedure; (2) the technique based on thermodynamic targets and physical insights as exemplified by pinch analysis; and (3) the algorithmic approach that utilizes optimization based on the construction of a superstructure that seeks to represent all feasible process flowsheets (Seider et al. 2009).

The intricate complexities associated with process synthesis problem in general and the refinery design problem in specific necessitates the development and implementation of a systematic and automated approach that efficiently and rigorously integrates the elaborate interactions involving the design decision variables.

*Model-Based Optimization for Petroleum Refinery Configuration Design*, First Edition. Cheng Seong Khor.

This work aims to extend the superstructure optimization-based approach of using logical constraints (Raman and Grossmann 1991, 1992, 1993a,b) within a MILP to incorporate qualitative design knowledge based on engineering experience and heuristics in modeling the major process flows in a refinery. These constraints adopt discrete integer decision variables of the binary 0–1 type to model the existence of a refinery process unit and the associated stream piping interconnections (which are effectively pipelines) in a network structure, in which a value of one for a 0–1 variable designates that a unit is present in the optimal structure while the converse is true for a value of zero.

Our work serves to further substantiate that the use of 0–1 decision variables offers a more natural and powerful modeling approach compared to the conventional linear programming technique that employs only continuous decision variables. It also affords the convenience of representing fixed-cost charges in the objective function formulation. A variation in the use of integer variables in optimization model formulations has been widely reported (Williams 1999).

Optimization is the core objective of chemical process design as exemplified through the synthesis of petroleum refinery configurations (Khor and Varvarezos 2017). Selecting the best among a set of possible solutions requires good engineering judgment to critically analyze the process with respect to the desired performance objectives. It is crucial to identify and strike a balance between the competing objectives of realizing the largest production, the greatest profit, the minimum cost, the least energy usage, and so on. This ensures improved plant performance through improved yields of valuable products, higher processing rates, longer time between shutdowns, and reduced maintenance costs. In order to find the best solution within the given constraints and flexibilities, a trade-off usually exists between capital and operating costs.

Although the design stage only takes up about 2% or 3% of a project expenditure, decisions made during this phase have an immense impact on plant economic performance because approximately 80% of the capital and operating expenses of the final plant are fixed during the design stage (Biegler et al. 1997). Hence, the necessity of developing systematic methods in chemical process design has led to two major strategies for process synthesis in determining an optimal configuration of a flowsheet and its operating condition.

In the first strategy, the problem can be solved in a sequential form involving decomposition, fixing some elements in the flowsheet, and then using heuristic rules to determine changes in the flowsheet that may lead to an improved solution. An example of such a strategy is the sequential hierarchical decomposition strategy by Douglas (1985, 1988). However, the sequential nature of the decisions and the heuristic rules that are used can lead to suboptimal designs. Douglas claims that only 1% of all designs are ever implemented in practice and hence this screening procedure avoids meticulous evaluation of most alternatives. It is not possible to rigorously produce an optimal design because the sequential nature of flowsheet synthesis cannot take all interactions among the design variables into consideration. Furthermore, the exponential number of possible topologies coupled with the multitude of process technology options decrease the chances of realizing the best design.

The second strategy that can be applied to solve a process synthesis problem is based on simultaneous optimization using mathematical programming (Grossmann 1996). This strategy requires the postulation of a superstructure, which includes a set of equipment that are potentially selected in the final flowsheet and their interconnections. The equations pertaining to the equipment and their interconnectivity in addition to the operating condition constraints are formulated in an optimization model with an objective function that typically minimizes cost or maximizes profit. In particular, such a formulation requires discrete variables to represent the choices of equipment besides continuous variables on the process parameters (e.g. flow rates) with which the model becomes a mixed-integer linear or nonlinear program (MILP or MINLP). In this regard, Grossmann (1996) states that an advantage of mathematical programming strategy is that they can perform simultaneous optimization of the configuration (as described by the discrete decisions) and operating conditions (as described by the continuous decisions).

Designing a petroleum refinery configuration is challenging and complex. Many factors such as design specifications and structural specifications have to be considered and incorporated at the conceptual design stage to arrive at an optimum configuration of the refinery flowsheet (Khor et al. 2011). Hierarchical decomposition uses heuristics, shortcut design procedures, and engineering experience to develop an initial base case, but doing so is possibly time-consuming, whereas the result may not necessarily guarantee an optimal solution. Thus, developing or adopting an automated systematic procedure in the refinery configuration design endeavor can significantly improve the decision-making process. The task can be achieved via optimization or mathematical programming approach by representing the problem through a superstructure and formulating the corresponding optimization model, which is solved to obtain an optimal configuration based on inputs of crude oils to be processed and final products to meet market demands while complying with the requisite constraints.

Figure 1.1 shows the rapidly rising downstream capital cost index from 2005 to 2019. Thus, an automated approach that can guarantee an optimal refinery design is increasingly important and sought after in the face of increased capital costs, higher energy costs, and depleting resources. At the same time, heightened fuel consumption leads to raised demand for petroleum products despite tight supplies with the consequential need to construct new grassroots petroleum refineries.

With increasingly stricter environmental regulations and emphasis on clean fuels, new refineries need to adhere to narrower operating margins and more stringent product specifications. This situation adds to the degree of complexity in designing refineries, which at present is already time-consuming with the intricacies of the interplay among the various factors including public opinions and permitting processes. All these considerations give rise to an exponential number of possible refinery topologies or configurations that can adequately meet current economic, operating, and environmental requirements.

We consider the following superstructure optimization problem for a refinery topology design. Given the following data: fixed production amounts of desired products, available process units and ranges of their capacities, and cost of crude oil

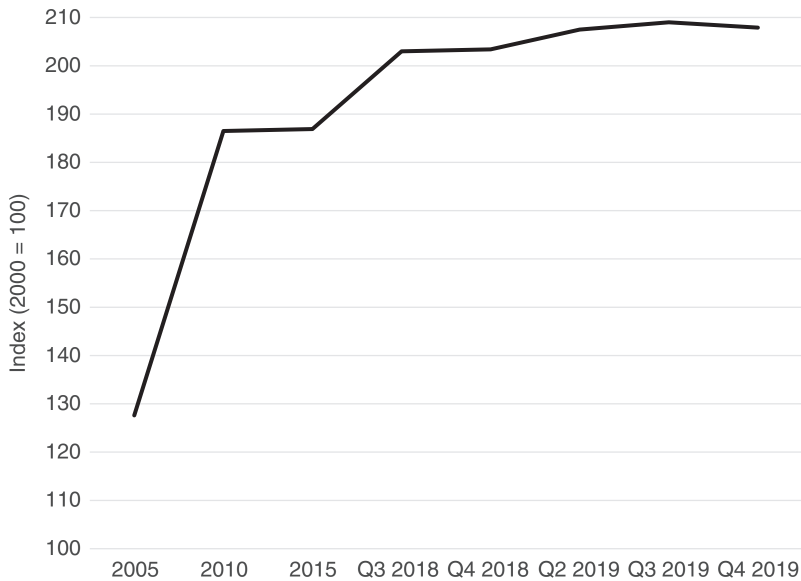



**Figure 1.1** Downstream capital cost index. Source: Data taken from Oil & Gas Journal (Editorial) (2019).

and process units, we wish to determine an optimal configuration in terms of the unit selection and sequencing as well as the operating levels.

This work aims to present a primer on superstructure optimization by emphasizing the following aspects:

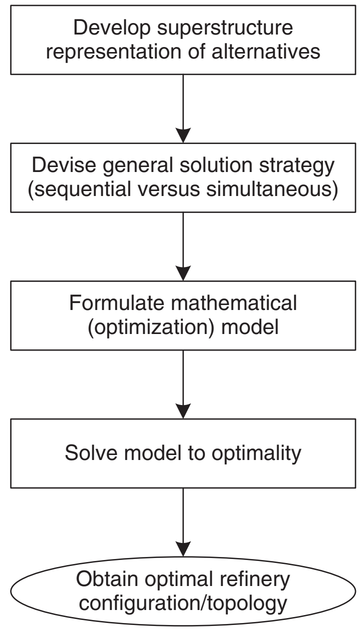
- developing a superstructure representation for a refinery network topology with a suitable level of detail;
- formulating models based on the superstructure representation by adopting two mixed-integer optimization frameworks: MILP and GDP, which incorporate both continuous and discrete decisions;
- solving the models using standard commercial off-the-shelf solvers enhanced with tailored solution strategies;
- analyzing and interpreting the model solution in terms of practical real-world applications.

A high-level view of the modeling approach adopted is shown in Figure 1.2.

## 1.2 Overview of Refining Processes

Petroleum products are made from crude oil. There are many types of crude oil from many different sources around the world. The selection of the right crude oil is a key part of the refining process. The decision as to what crude oil or combination of crude oils to process depends on many factors including quality, availability,

**Figure 1.2** Flow chart on modeling methodology.




volume, and price. Table 1.1 briefly describes functions of several major refinery processes (Figure 1.3).

### 1.2.1 Atmospheric Crude Oil Distillation

The first stage of crude oil processing involves distillation or fractionation. The crude oil is distilled into fractions according to boiling point to yield light-end hydrocarbons ($C_1$–$C_4$), light naphtha, heavy naphtha, kerosene, diesel, and atmospheric residual. Some of these broad cuts can be marketed directly, while others require further processing in downstream units. Increased efficiency and reduced costs are achieved if the crude oil is fractionated at essentially atmospheric pressure followed by residue or bottoms fractionation using vacuum distillation (Figure 1.4).

Naphtha is a complex mixture of paraffins, naphthenes, and aromatics in the range of five-to-twelve carbon molecules ($C_5$–$C_{12}$). Straight-run naphtha is obtained directly from the atmospheric distillation unit. Light naphtha is the fraction boiling from 30 to 90 °C and contains $C_5$ and $C_6$ hydrocarbons. Heavy naphtha is the fraction boiling from 90 to 200 °C and contains $C_7$–$C_9$ hydrocarbons, which is the favored feedstock to the catalytic reformer. Naphtha can also be sourced from the processing of heavier crude fractions in visbreaker, catalytic cracker, hydrocracker, and coker in which olefinic hydrocarbons are present (Speight 2011).

### 1.2.2 Hydroprocessing

Hydrotreatment is the conventional means for removing sulfur from petroleum fractions. This process is important to avoid poisoning of the reformer catalyst and

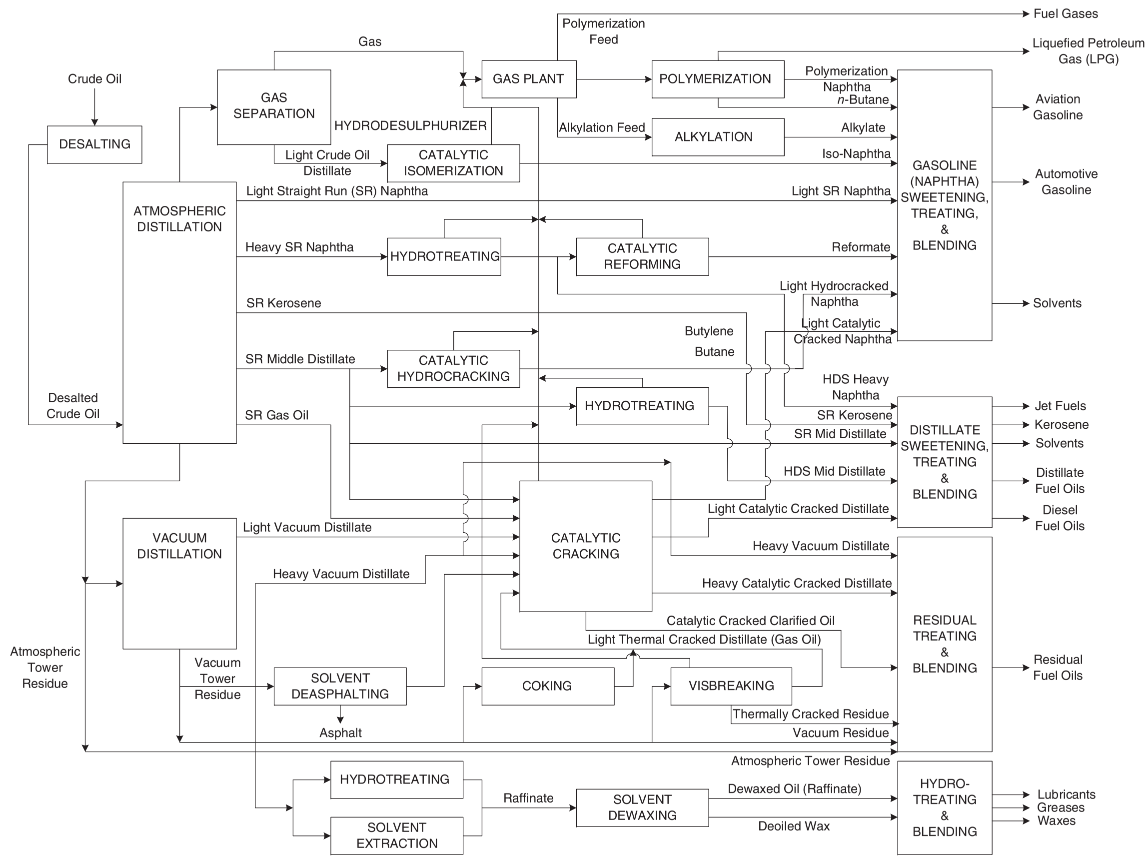



**Figure 1.3** Refinery process flow. Source: Adapted from Speight (2011).

**Table 1.1** Functions of major refinery processes.

| Process unit | Function |
|---|---|
| Atmospheric distillation unit (ADU) | Initial separation of crude oil into the raw products of light gases, naphtha, kerosene, and diesel with the resulting residue of the atmospheric bottoms stream |
| Naphtha hydrotreater (HDT) | Uses hydrogen to desulfurize naphtha from atmospheric distillation, which must be hydrotreated before being sent for catalytic reforming |
| Catalytic reformer (REF) | Convert naphtha-boiling range molecules into higher octane reformate (i.e. reformer product) that has higher content of aromatics and cyclic hydrocarbons; an important byproduct is hydrogen released during reaction which is used either for hydrotreating or hydrocracking |
| Fluid catalytic cracker (FCC) | Upgrades heavy petroleum fractions into more valuable lighter products |
| Hydrocracker (HCR) | Uses hydrogen to upgrade heavier fractions into more valuable lighter products |
| Visbreaker (VIS) | Upgrades heavy residual crude oils by thermal cracking into more valuable lighter products with reduced viscosity |
| Coker (COK) | Converts very heavy residual crude oils into gasoline and diesel fuel with petroleum coke as residual product |
| Isomerizer (ISO) | Converts linear petroleum molecules to higher-octane branched molecules for gasoline blending or as alkylation feed |
| Alkylation unit (ALKY) | Reacts low molecular-weight olefins with an isoparaffin to form higher molecular-weight isoparaffins |

to meet environmental legislations on combustion gas emissions. The feedstock is passed together with hydrogen-rich gas (usually above 75% of hydrogen by mass), over a fixed bed of catalyst under conditions that depend mainly on the feedstock properties and desired product specifications. Hydrodesulfurization consumes hydrogen and generates hydrogen sulfide according to the general reaction:

$$\mathrm{R{-}S{-}R} + 2\mathrm{H_2} \rightarrow 2\mathrm{R{-}H} + \mathrm{H_2S}$$

where R represents an alkyl group and S represents a sulfur atom. The severity of a hydrotreater depends on the amount and types of sulfur compounds in the naphtha feed, which in turn are determined by the crude oil source. Characterization of sulfur compounds in naphtha is particularly difficult due to extremely low concentrations. The sulfur composition in a blend (60% straight run and 40% hydrocracked naphtha) is almost the same as straight-run naphtha since sulfur contribution from hydrocracked naphtha is negligible (Ali 2004a).

Catalytic naphtha hydrotreatment can simultaneously accomplish desulfurization, denitrogenation, and olefin saturation. Lower boiling compounds are desulfurized more easily than high boiling ones. Reactivity decreases with increasing

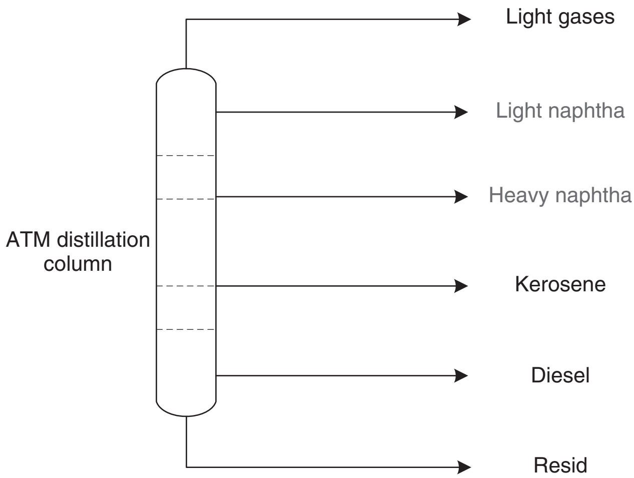



**Figure 1.4** Fractions from atmospheric crude distillation unit.

**Table 1.2** Naphtha hydrotreater: typical yields.

| Component | | Yield (weight) |
|---|---|---|
| Feed | Naphtha | 1.0000 |
| | $H_2$ | 0.0080 |
| | Total | 1.0080 |
| Products | Acid gas | 0.0012 |
| | $H_2$-rich gas | 0.0110 |
| | LPG-rich gas | 0.0058 |
| | Desulfurized naphtha | 0.9900 |
| | Total | 1.0080 |

molecular size. Products from the naphtha hydrotreater are generally acid gas, hydrogen-rich gas, liquefied petroleum gas- or LPG-rich gas, and desulfurized naphtha. Table 1.2 presents the typical yields in terms of weight fraction for feed and products of a naphtha hydrotreater (Parkash 2003c). The desulfurized naphtha from the hydrotreater can also be categorized as light and heavy.

The hydrodesulfurization of organosulfur compounds is exothermic. The amount of heat released increases with the number of moles of hydrogen consumed. This heat of reaction can increase the reactor temperature by 10–80 °C at nominal operating conditions depending on the feedstock (Ali 2004b). The conditions typically used to hydrotreat straight-run feedstock are mild, whereas treating cracked feeds (or blends of cracked and straight-run feeds) requires more severe conditions. The main operating variables are temperature, hydrogen partial pressure, and space velocity. In general, an increase in temperature and hydrogen partial pressure increases the

**Table 1.3** Sulfur recovery unit yields.

| Component | | Yield (weight) |
|---|---|---|
| Feed | $H_2S$ gas | 1.0000 |
| | Total | 1.0000 |
| Products | Sulfur | 0.8478 |
| | Loss | 0.1522 |
| | Total | 1.0000 |

reaction rates of sulfur and nitrogen removal, while an increase in space velocity has the reverse effect.

### 1.2.3 Sulfur Recovery

The hydrogen sulfide generated in the hydrotreater is sent to sulfur recovery unit before it is burnt as refinery gas. The conversion of hydrogen sulfide to elemental sulfur is necessary to minimize atmospheric pollution by sulfur dioxide. This is in line with environmental regulations, which mandate the recovery of 99% or more of the sulfur in refinery gas (Gary and Handwerk 2001). Sulfur recovery unit operates based on the Claus process, which proceeds as follows:

$$\text{Burner: } 2H_2S + 3O_2 \rightarrow 2H_2O + 2SO_2$$

$$\text{Reactor: } 2H_2S + SO_2\ 2H_2O + 3S$$

One-third of the $H_2S$ is converted to $SO_2$ by combustion, which is then combined with the remaining two-thirds and passed over a catalyst where molten sulfur forms and is separated from the gas stream. This sulfur is sold to generate additional revenue. The gas stream is cooled by steam generation and passed over another catalyst bed. This cycle is repeated for as many as four catalyst beds in some instances. The gas stream leaving the sulfur recovery unit still contains $H_2S$ and/or $SO_2$, which requires further treatment. Table 1.3 shows the product yields from a sulfur recovery unit (Parkash 2003d).

### 1.2.4 Reforming

The continuous demand of today's automobiles for high-octane gasoline has stimulated the use of catalytic reforming to produce high-octane reformate from desulfurized naphtha without changing the boiling point range, as well as to provide hydrogen required for hydrotreating. The typical feedstocks to reformers are heavy straight-run naphtha and heavy hydrocracker naphtha. These are composed of four major hydrocarbon groups: paraffins, olefins, naphthenes, and aromatics (also referred to as PONA). The main function of a reformer is to convert paraffins and naphthenes into aromatics, subsequently producing high-octane reformate. Typical

**Table 1.4** Catalytic reforming: feedstocks and products.

| RON Component | Feed (vol%) | Product (vol%) |
|---|---|---|
| Paraffins | 30–70 | 30–50 |
| Olefins | 0–2 | 0–2 |
| Naphthenes | 20–60 | 0–3 |
| Aromatics | 7–20 | 45–60 |

reformer feedstocks and products have the PONA analyses shown in Table 1.4 (Gary and Handwerk 2001).

Paraffins and naphthenes undergo two types of reactions in being converted to higher octane components: cyclization and isomerization. The ease and probability of either of these reactions occurring increases with the number of carbon atoms in the molecules. It is for this reason that only heavy straight-run naphtha is used for reformer feed. Light straight-run naphtha is largely composed of lower molecular weight paraffins that tend to crack to butane and lighter fractions, thus uneconomical to process in a catalytic reformer. Hydrocarbons boiling above 204 °C are easily hydrocracked and cause an excessive carbon laydown on the reforming catalyst.

The desirable reactions in a reformer that lead to forming aromatics and iso-paraffins mainly involve the following: (1) isomerization of *n*-paraffins to iso-paraffins, (2) dehydrocyclization of paraffins to aromatics, (3) dehydrogenation of naphthenes to aromatics, (4) saturation of olefins to form paraffins which then react as in isomerization in reaction (1.1) and dehydrocyclization in reaction (1.2); aromatics are essentially left unchanged (Maples 2000). Undesirable reactions are dealkylation of side chains of naphthenes and aromatics besides the cracking of paraffins and naphthenes. Table 1.5 shows typical reformer yields for three values of research octane number (RON) (Parkash 2003a).

### 1.2.5 Isomerization

The octane numbers of light straight-run naphtha can be improved by isomerization to convert normal paraffins of $C_5$ and $C_6$ to their isomers. This operation results in a significant octane increase because *n*-pentane has a RON of 61.7, whereas the RON of iso-pentane is 92.3 (Gary and Handwerk 1994).

Equilibrium conversion to isomers is enhanced at lower temperatures, hence a reactor temperature of 98 to 205 °C is desirable. At these low temperatures, a very active catalyst is necessary to provide a reasonable reaction rate. Catalysts used for isomerization contain platinum on various bases. Small amounts of organic chlorides are injected continuously to maintain high catalyst activities. This leads to the formation of hydrogen chloride in the reactor, which necessitates the feed to be free of water and other oxygen sources so that catalyst deactivation and potential corrosion problems can be avoided. An atmosphere of hydrogen is used to minimize carbon deposits on the catalyst but hydrogen consumption is negligible (Gary and

**Table 1.5** Catalytic reforming: typical product yields in weight fraction.

| RON<br>component | 96 | 100 | 102 |
|---|---|---|---|
| $H_2$ | 0.0193 | 0.0310 | 0.0320 |
| $C_1$ | 0.0085 | 0.0120 | 0.0140 |
| $C_2$ | 0.0138 | 0.0200 | 0.0230 |
| C | 0.0269 | 0.0290 | 0.0330 |
| $iC_4$ | 0.018 | 0.0170 | 0.0190 |
| $nC_4$ | 0.0228 | 0.0230 | 0.0260 |
| $iC_5$ | 0.0276 | — | — |
| $nC_5$ | 0.0184 | — | — |
| $C_5$+ | — | 0.8680 | 0.8530 |
| $C_6$+ | 0.8447 | — | — |
| Total | 1.0000 | 1.0000 | 1.0000 |

**Table 1.6** Isomerization yields.

| Component | | Yield (weight fraction) |
|---|---|---|
| Feed | Light naphtha feed | 1.0000 |
| | Hydrogen | 0.0040 |
| | Total | 1.0040 |
| Products | Isomerate | 0.9940 |
| | Gases | 0.0100 |
| | Total | 1.0040 |

Source: Data from Parkash (2003b).

Handwerk 1994). Slight hydrocracking occurs during isomerization, resulting in loss of gasoline and production of light gases. Light straight-run naphtha is also sold as petrochemical feedstock besides being sent to the isomerization unit. Table 1.6 shows typical isomerization yields.

### 1.2.6 Blending

The final stage of the refining process is blending. This is a crucial step where the various hydrocarbon components manufactured in the refinery are mixed together to make the final products sold by the refinery. The final blend recipes depend on the quality of the available components and on customer requirements or specifications. All blended products are tested before they are sold to ensure that they meet the specifications.

## 1.3 Overview of Refinery Optimization Modeling

The refinery design process can be described as consisting of three stages, namely, synthesis, analysis, and optimization.

- Synthesis involves identifying the possible need for a product, e.g. by conducting market feasibility study.

### 1.3.1 Refinery Optimization Systems, Techniques, and Tools

A wide range of model-based systems and tools, typically computerized with associated modeling strategies, are now pervasively available and increasingly used to help design refineries in meeting desired requirements and intended applications. As depicted in Figure 1.5, the major model-based related (or assisted) elements are briefly described as follows (Engell 2007):

- regulatory control supported or enhanced with advanced process control (APC) techniques such as the popular model predictive control (MPC) systems;
- real-time optimization (RTO) that can be implemented for both static (i.e. steady state with certain criteria for such a certification, which is the typical or traditional practice) and dynamic conditions;
- instrumentation such as sensors, analyzers, and actuators which deliver digital information at an enhanced rate;
- programmable logic controllers (PLC), distributed control systems (DCS), personal computers, and real-time servers, which are now considerably inexpensive, thus more available to buy (even in excess of required capacities) and maintain;
- new online analysis technology (including analyzers) such as near-infrared spectroscopy (commonly known by its abbreviation of NIR);
- software that supports devices, systems, and technologies enabled by (Industrial) Internet-of-Things or more popularly abbreviated as (I)IOT, which capitalizes on the capability afforded by the Internet including high-performance tools for storing and accessing data (e.g. in the cloud or at the edge);
- new tools as means of communication that are increasingly rapid and reliable from transmitting initial input data up to integrating with management level (e.g. at the headquarters);
- software development efforts that are continually reducing the need for proprietary modeling systems requiring the expertise, knowledge, or skills of a specialist;
- new powerful computational concepts, methods, and techniques for model development and solution such as machine learning (e.g. neural network), which has gained a lot of attention recently (besides mathematical programming, constraint programming, fuzzy logic, or others).

A number of commercial optimization tools are routinely used in the industry that typically include the following:

- PIMS (Process Industry Modeling System by Aspen Technology): Technique called sequential linear programming (SLP) augmented with recursion methods

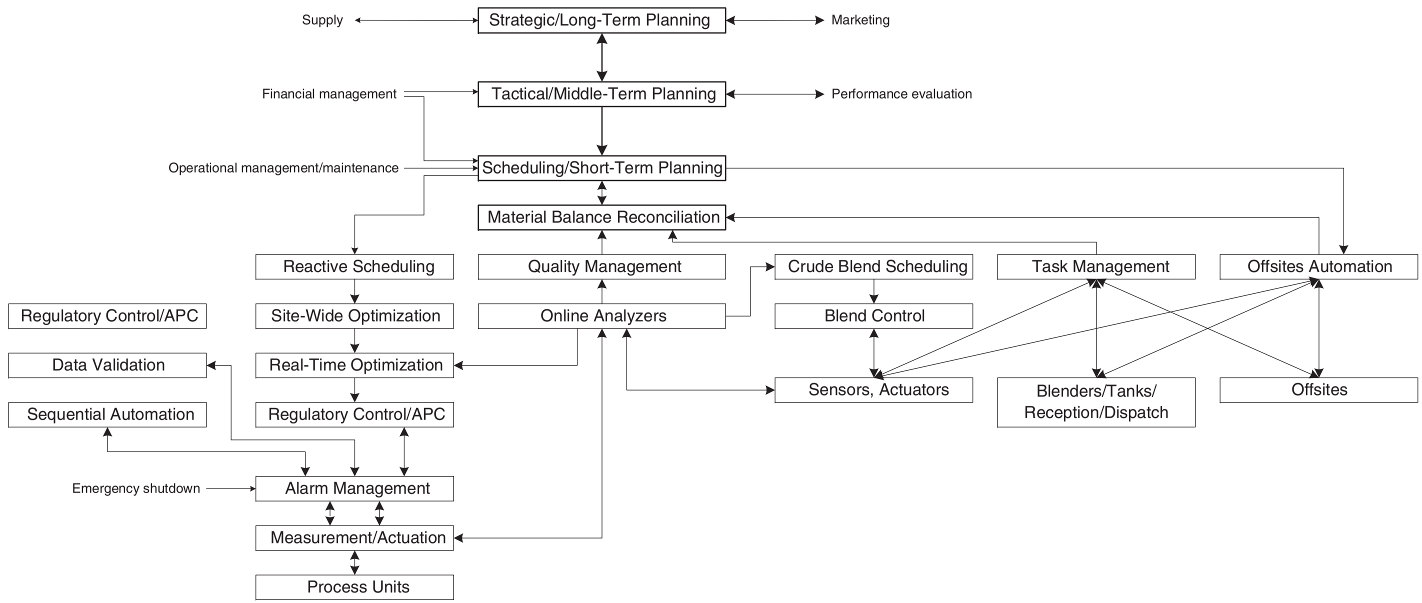



**Figure 1.5** Model-based related elements for typical refinery decision-making support systems.

is employed to enable handling some nonlinear functions (e.g. bilinear terms that arise due to mixing process operations) through an iterative procedure; spreadsheet-based user interface; and reporting;
- Excel Solver (add-in by FrontLine used in Microsoft Excel): Uses spreadsheet format for inputs/outputs;
- Sequential quadratic programming (SQP) as employed (also pioneered) through the deployment of dynamic matrix optimization (DMO) technique: Uses algorithm based on derivatives of functions to search for optimality; equations are written in standard Fortran format with extensive linking to execute optimization functionalities.

### 1.3.2 Modeling for Advanced Process Control

APC is an area that has long experienced a widespread practice of implementing model-driven or model-assisted technology (Lee et al. 2018). APC applications in refineries are mainly concerned with real-time multivariable control as based on (largely) empirical models of process units. Such models can be incorporated with dynamic RTO to improve the setpoints computed for implementation in APC, most commonly through applying MPC systems (Kadam and Marquardt 2007; Pontes et al. 2015).

The availability of sufficient degrees of freedom for modeling, control, and optimization supported by excellent instrumentation for measurements has allowed refineries to benefit significantly from these model-based techniques and tools. The advantages can be exemplified (in whole or part) through easier, faster, safer, and even greener (i.e. more environmental friendly) process unit management afforded by more effective response. The resultant stability of operating conditions also improves handling of changes in the production environment such as variations in feedstock quality and weather conditions.

Consequently, these granted refinery operations to maximize throughput of higher feed flow rate resulting from being able to push multiple process constraints in an optimal manner to higher levels. At the same time, increased process capability due to reduced process variabilities permitted higher stream yields in meeting market demands particularly for high-value products. As a result, refineries improve energy and general operation efficiency through less consumption of utilities and chemicals as well as catalysts, lower losses due to manufacturing-related issues; and decreased fluctuations in quality and the associated giveaways in product properties.

Modeling using APC contributes significantly to a large part of the potential benefits derived in which the benefits can be quantified from refinery revamp projects. Thus it is prioritized to carry out such value-improvement projects. Some of the popular commercial APC software systems widely used in refineries worldwide include Aspen Technology's DMC (which historically stands for Dynamic Matrix Control) and Honeywell's Robust Multivariable Predictive Control Technology (RMPCT) (Morari and Lee 1999). Trade information up-to-date on currently operating APC systems is available in references such as Hydrocarbon Processing, a monthly periodical which also publishes an annual supplement (called Advanced Process Control and Information Systems Handbook).

APC has been a mainstay in the refinery suite of modeling tools and applications for the past two decades or so (Forbes et al. 2015). In comparison, optimization modeling tools for online (real time) or offline purposes have not been used as commonly, extensively, or pervasively relative to APC although arguably the trend has gained more widespread acceptance in more recent times (Lee 2011).

Despite its many advantages, a possible objection to APC is that even erroneous setpoints are simply implemented quickly when the most difficult part of refinery operations is to ensure that setpoint values as accurate as possible are established in the automated controls. Thus, RTO, also known as online optimization systems, is employed for determining the optimal values for the setpoints sent to the APC by executing online calculations (as briefly reviewed next).

### 1.3.3 Modeling for Real-Time Optimization

Compared to APC, there are relatively fewer commercial RTO applications; even less common is a plantwide operational optimizer (with the level of detail as that of a typical RTO), which is currently used in the downstream petroleum processing industry. Conventional RTO models are required to generate solutions within minutes of execution (after achieving steady state as determined by certain appropriate criteria). At the same time, the models are updated with economic and technical conditions data of process units in a continuous and automated way. The latter necessitates reliable and reasonably fast digital systems capable of collecting and validating the data including to verify steady-state conditions in developing the processing unit flowsheeting models.

In a similar way, a number of process simulation packages incorporate RTO-like features of general optimization capabilities in addition to offering combined or hybrid first-principle and empirical modeling options. Since the models used for the optimization must be able to integrate all of the system's constraints and use the degrees of freedom available, the resulting optimization models formulated can be complex. The complexity is manifested particularly by the requirement to handle over hundreds of thousands of equations in which some are possibly nonconvex (e.g. bi-/tri-linear or exponential) as well as millions of variables, all subject to a simultaneous solution strategy to be devised and executed in arriving at some meaningful (if not practical) results.

It is noteworthy that a standard rigorous approach of RTO-based modeling typically involves the following sequential procedure (as summarized in the flowchart shown in Figure 1.6). The first step involves periodically executing an algorithm, which is generally based on nonlinear optimization that gathers data from steady-state operations. The second step performs data reconciliation between the actual plant and model values. The third step consists of adapting or updating some model parameters so that the model results match the reconciled data to an acceptable degree of accuracy. The fourth step computes optimum target values as improved setpoint candidates for identified (i.e. preselected or preconfigured)

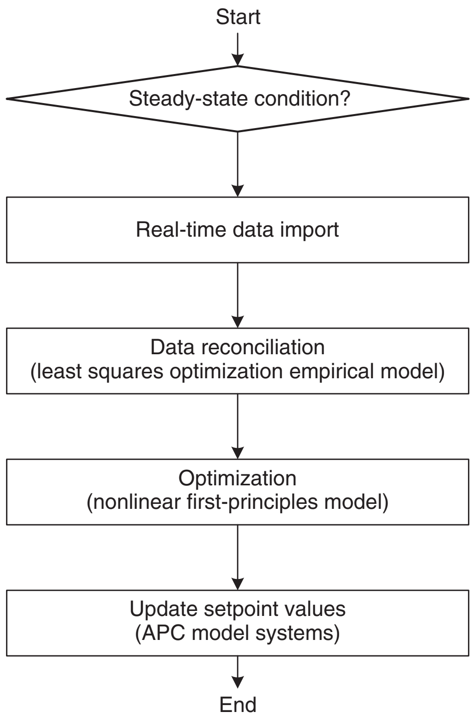



**Figure 1.6** Standard cycle procedure for typical real-time optimization modeling systems (online and closed loop).

process variables as handles to optimize (mainly for local optima) the process units or the entire refinery in general. The final step entails modifying by implementing the necessary process setpoints. The cycle is then repeated when a steady-state criterion is verified to be attained (Bodington 1995; Moro 2003).

Recent developments in the petroleum refining world include efforts to implement simultaneous optimization of models for multiple units in real-time mode. An ultimate goal is to enable online economic optimization (i.e. with commercial significance or impact) of the total refining process from the front-end (including berth- or dock-related activities) to the back-end (including end-products distribution). A crucial enabler for successful applications to problems of industrial scale and significance is the availability of powerful nonlinear optimization algorithms (de Prada et al. 2017).

Conventional RTO software packages are equation-oriented systems that make use of robust large-scale nonlinear programming algorithms as the solution engine (e.g. SQP) such as the implementation in the commercial package called ROMeo (Rigorous Online Modeling with equation-based optimization) (AVEVA 2021). A user can expect to find in an RTO package such standard features like combination of the underlying mathematical formulation and solution engine with an interface (typically GUI or graphical user interface). The combined components of the package or systems are designed to capture and show real-time plant data and economic objective function values, which attempt to depict a replica (i.e. a model) of the plant operations in as close as possible a manner.

A modeling-aided management system such as RTO, which is coupled to APC offers a capability that allows users (i.e. plant engineers as well as the management besides the modelers especially those personnel at the site) to have a reliably rigorous, precise, and accurate model of the process units in an operating facility to optimize operations on a plant-wide basis by determining optimal process setpoints for the plant control systems. In doing so, such a model-based system also assists in determining the cause and source (or location) in which operating bottleneck problems and challenges lie. A single model with a modern user-friendly GUI approach (such as that in the manner of RTO), instead of separate models catering for multiple uses including process simulation, data reconciliation, and operational optimization, facilitates to develop, deploy, and sustain a model with reduced cost.

Notwithstanding significant continuous progress as mainly found reported in both trade periodicals and academic journals, which includes a recent partnership between AVEVA and ExxonMobil Research and Engineering Co. (EMRE) to enhance ROMeo's capability, it remains arguable that RTO still lacks general industrial acceptance (not least, relative to APC). The reasons could be due to certain practical and also theoretical limitations. Some of these drawbacks generally pertain to the levels of detail in characterizing the feed streams, developing the process unit models, and detecting the existence (or nonexistence) of true steady state (the latter applies particularly to plants with reasonable disturbance).

Nonetheless, substantial noteworthy effort has been undertaken to address these issues for both the system modeling as well as the solution parts of RTO technology. Improvements are partly reflected from industrial implementations of RTO particularly for ethylene processing plants for petrochemical production besides the petroleum refining industry (Shobrys and White 2000; Moro 2003; Karuppiah and Grossmann 2006). Nonetheless, existing commercial RTO packages have been thought of as somewhat dated (notwithstanding ongoing modernization initiatives to incorporate state-of-the-art features, which include utilizing cloud and edge computing technologies). Some examples along this line are exemplified in packages enabled by dynamic optimization-based modeling and solution techniques such as gPROMS software by Process Systems Enterprise (now owned by Siemens) or GDOT software by Aspen Technology (now owned by Emerson).

### 1.3.4 Modeling for Process Simulation

Commercial model-driven process simulators are now largely considered as a common omnipresent basic available tool required to enable and assist refinery process engineers mainly to perform detailed material and energy balances. Subsequently, the results (mostly available for steady-state condition but increasingly also for dynamic condition) are requisite for a variety of other tasks and purposes as part of design, operation or production, and maintenance or sustainment support activities. Some examples of the latter (i.e. for maintenance applications) are more and more used for debottlenecking studies on unit operations for plant revamp and rejuvenation exercises.

Notable examples of general-purpose simulators include Aspen Plus (Aspen Technology 2021b); UniSim (Honeywell 2021); VMGSim (Virtual Materials Group (VMG) 2021) for which different versions have been customized (called iCON for PETRONAS, the Malaysian national oil company) and now acquired by Schlumberger (called Symmetry); PRO/II (formerly of Invensys and now acquired by Schneider Electric); and Petro-SIM (formerly of KBC and now acquired by Yokogawa). A number of these packages also offer tailored or bespoke detailed models for specific refinery processes such as fluidized catalytic cracking (FCC), catalytic reforming, and hydrocracking. On the other hand, commercial specialized simulation tools are also available to perform realistic simulation-based modeling for certain process units in which detailed diagnostic studies are necessary. In this realm, some of the examples pertaining to refinery-based applications include those that need to incorporate detailed reaction kinetics in the modeling of conversion units particularly for catalytic reforming, FCC, and hydrocracking units.

In addition, process simulation have been integrated as part of the routines in certain plant optimization models. Such integration are performed in either online or offline mode—typically the former is executed on continuous real-time basis while the latter on longer-term advisory or study basis. These integrated models typically employ the latest process information extracted or imported from process simulation models to update existing process plant models (Hallale et al. 2006).

As an example, Aspen Technology, a perennial market leader in provisioning of modeling and optimization software, systems, and support services particularly for refinery planning and scheduling, has extended its models to make available detailed reactor representation with rigorous kinetics modeling for optimizing hydrogen production (Aspen Technology 2021a). Such models, which are dubbed as hybrid models since they combine both first-principles and empirical modeling techniques coupled with artificial intelligence and analytics algorithms, have enabled a better understanding of process operations under different hydrogen feed conditions. The hybrid reactor simulation models developed in AspenPlus can also be linked to and employed in Aspen PIMS with automatic updates available, thus allowing the combined models to perform enhanced detailed planning and scheduling activities as well as economic evaluation (Beck and Munoz 2020).

#### 1.3.4.1 Modeling for Dynamic Simulation

A related development concerns modeling for dynamic process simulation. Several software packages have resulted from more than three decades of research and development (R&D) intertwined with systems design or customization. Applications of unit-wise and plant-wide dynamic simulation can be readily adopted as part of an extensive modeling suite now available to assist with optimal decision-making in refinery operations. Some examples of early equation-based modeling software systems include DIVA (Kröner et al. 1990), ABACUSS (Allgor et al. 1996), and SPEEDUP (Perkins and Sargent 1982) – the latter forms a base that has been further developed and evolved to be a state-of the-art current cutting-edge package called gPROMS (Barton and Pantelides 1994) by Process Systems Enterprise (a spinoff company of Imperial College London's Department of Chemical Engineering, which since has been acquired by Siemens) (Siemens 2021).

Such large-scale dynamic system simulation software allows a modeler or an engineer to focus solely on formulating and thereafter implementing the model developed. An advantage of doing so is that it generally removes or obviates the modeler/engineer from concerns about solution algorithms (such as infeasibility due to numerical issues caused by parameter or variable scaling) and code-related issues (such as syntax for generation, compilation or interpretation, and debugging). This modeling aid greatly permits the modeler/engineer to increase productivity while assisting to ensure the dynamic simulation feasibility. Relevant activities regarding such refinery use include designing, verifying, and analyzing parametric sensitivity for control and safety interlock systems as well as investigating operational events of start-up, changeover, and shutdown.

#### 1.3.4.2 Modeling for Operator Training Simulation

Refinery training simulators based on dynamic simulation modeling technique (as discussed in Section 1.3.4.1) are now an essential tool to train new operators especially panel operators manning the control rooms besides to maintain and update the operators' knowledge and skill regularly in reacting to exceptional circumstances. Although (panel) operators now are exposed to operational incidents much less frequently than in the past (mainly due to control room reorganization), the increased scope, level, and reliability of automation (which is also partly exacerbated by the Covid-19 virus outbreak pandemic) have led to requirements for increased duration and alternative suitable methods for operator training. Thus to guarantee a refinery's safety in the situation of automation systems failure, which can lead to plant failure altogether, it is imperative to enhance operators' readiness through enhanced training level including by adopting a model-based approach.

We can represent realistic operating conditions using dynamic simulation models in a manner akin to how flight simulators are used for aircrew training (e.g. for civilian aircraft or military air force). The similarity of the roles is particularly apparent to allow modeling of transient time period in the event that follows after an incident or operational change. We can also expect state-of-the-art dynamic simulators to be able to model several possible scenarios including to evaluate historical data of past operator's real-time reactions.

Models for training simulators typically include operator consoles (which are identical to those one may expect to see in the control rooms) as a feature linked to the DCS. Modeling in this way enables access to initial states of the process variables. Indeed, training simulators and their comprehensive use are a showcase of modeling capability in supporting high competence of safety assurance in refinery operations.

### 1.3.5 Modeling for Planning and Scheduling

Modeling of refinery planning and scheduling serves to represent, predict, and prescribe the establishment of a detailed manufacturing activities plan for a plant across various time scales (ranging from seconds or minutes up to several years). Planning and scheduling enable and support enterprise supply and marketing functions of a company by defining specific activity timings in producing the requisite product volumes that fulfill the company's objectives. Based on requirements stipulated by the company operations, the main goal of refinery planning and scheduling is in meeting the demands of primary outlets of national and international retail sales (Pompéi 2001). A side goal of the production plans and schedules also serves to minimize any associated byproducts generated since typically they are of uneconomical values.

Thus, modeling for refinery planning and scheduling systems is vital particularly to improve feeds as throughput to the process units in realizing potential large returns or margins and saving costs significantly. But a main complicating challenge in modeling refinery operations lies in representing the operation modes of the process units involved, i.e. that can be not only mostly continuous in nature but also batch or semi-batch (or semi-continuous). Such operating considerations are on top of a need to deal with the existing complexity involved in handling the various crude oils feed mix and product grades. In addressing these issues, the modeling effort entails adopting both the more conventional continuous and discrete types of decision variables and the corresponding constraints as adequately espoused elsewhere (Karuppiah et al. 2008). Doing so allows modeling with greater flexibility besides incorporating practical problem representation in the model formulation as will be illustrated throughout the book.

As shown in Figure 1.7, planning and scheduling activities in a refinery are made up of several sections. These sections can be represented conveniently as separate modules of optimization models, namely, crude oil movement and blend scheduling (at the refinery front-end), production planning and scheduling (refinery middle-end), and product blending and distribution scheduling (refinery back-end) (Jia and Ierapetritou 2003; Reddy et al. 2004; Méndez et al. 2006).

The front-end plans and schedules involve blend scheduling optimization of crude oil mixtures (i.e. crudes for short) that include handling arrival events of crudes such as unloading from vessels, transfer to storage tanks, and blending and charging of crudes as feedstock for processing in crude distillation units. The middle-end plans and schedules address process unit operations of the intermediate streams including their inventory control from one unit to another. The process operations involve reactions to modify and attain the desired output such as product properties (e.g. higher octane number) as well as separation to increase product purity (e.g. lower contaminant concentrations), which can entail a need for handling effluents. The back-end plans and schedules deal with product blending and dispatch or distribution in which the latter largely involves logistics optimization around end-products lifting for shipping delivery to customers (i.e. demand centers or points) and including inventory control that serves to prevent stock out.

Refinery commercial success depends to a great extent on how the associated plans and schedules are modeled for development, deployment, and sustainment. Thus, it is imperative for a refinery to be able to put in place a robust and reliable as well as automated process of modeling and computing in generating optimal or feasible plans and schedules. Typically, a database, e.g. one based on SQL

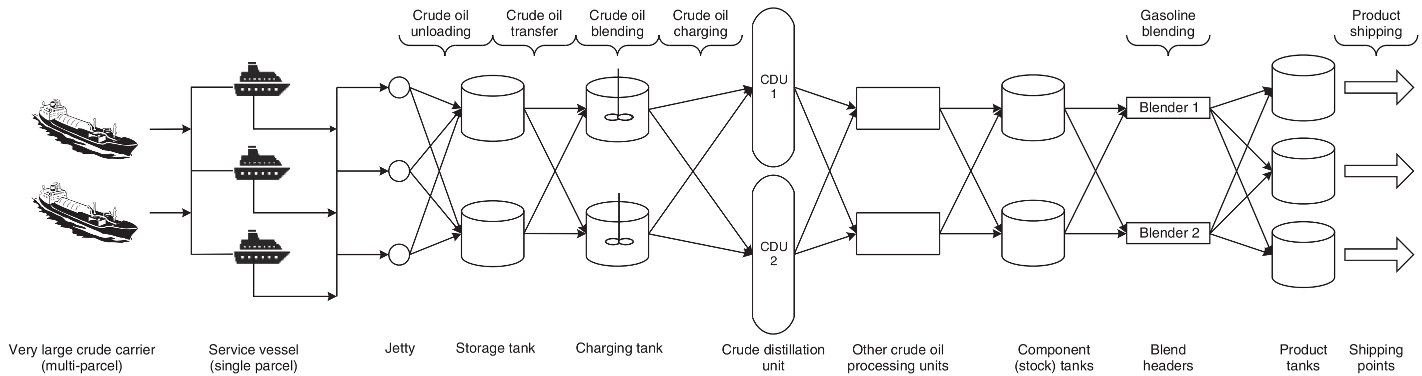



**Figure 1.7** Schematic for optimization modeling of refinery end-to-end encompassing crude oil blend scheduling (at front-end), process planning and scheduling (middle-end), and product blending and delivery (shipping) scheduling.

(structured query knowledge) is used particularly within a short-term scheduling model to ensure that a refinery implements the generated plans and schedules in a consistent manner between one to the other with the latter (i.e. results from the scheduling activity) involving more details or granularity than the former (i.e. results from the planning activity).

The consistency in data and its validity are ensured particularly on yields, costs, and throughputs. Such undertaking necessitates significant requisite effort in maintaining, establishing, and integrating the database with the refinery-wide information systems encompassing both IT (information technology) and OT (operating technologies) including management-centric dashboards.

In view of the drive for increased or enhanced digitalization spurred by the Industrial Revolution 4.0 (IR4.0) paradigm and the onset of the Covid-19 (coronavirus) pandemic, model-based tools for decision-making support systems have seen a surge of interests particularly but not limited to the activities of optimizing refinery plans and schedules. The actual situation is not something entirely new because even previously, refineries face amplified pressures constantly due to intensified operating challenges brought about by tightened market, regulatory, and environmental requirements (also sometimes referred to as the so-called "triple bottom-line") as well as heightened priorities for social and governance aspects.

Ongoing recent technical advances have generated renewed interests in computer-aided model-based decision-making tools to improve refinery planning and scheduling activities continually. In particular, the following refinery optimization developments have enabled more benefits to be reaped with increased speed and scale:

- greater operational complexity in raw materials handling due to pressures of attaining economic advantage of processing cheaper challenged crudes (with typically more diverse crude oil mixtures);
- quicker and more rapid supply chain responsiveness to market dynamics to capture more value;
- reduced operating degrees of freedom arising from a greater number of constraint, e.g. more stringent product specifications, stricter environmental requirements, and tighter tankage limitations;
- generally easier, faster, and more accurate (relatively) problem formulation through adopting increasingly powerful state-of-the-art modeling techniques (e.g. logic-based constraint programming, artificial-intelligence-based expert systems, and hybrids of mixed-integer optimization involving combined mixed-integer programming with disjunctive programming);
- by a similar token to the previous point (i.e. in the same way as afforded by the availability of more sophisticated models), more efficient solution and implementation or deployment of model-based optimization for decision-making support system;
- more advanced computing and computational capacity afforded by the increased availability of more powerful hardware and more efficient algorithms;
- massive refinery data availability (i.e. in terms of volume, velocity, variety, veracity, and value which collectively describes the "big data" phenomenon) as well as that

related to the parent company or enterprise networks, which has given access to requisite information instantly and pervasively through internet and web-based technologies or infrastructures (e.g. cloud computing or Industrial IoT components in general).

The situation has enabled complex planning and scheduling problems with solution methods and strategies that can cater for discrete decisions. Such models involve both continuous and integer (often binary) types of decision variables. Thus, the application necessitates handling an exponential number of feasible plans and schedules with their associated permutations. In particular, the mathematical formulation and model development undertaking give rise to combinatorial optimization of mixed-integer programming with tools and techniques that can now afford such problems to be solved within tractable and practical computational effort and execution or run time.

The techniques of advanced model-based optimization coupled with powerful and scalable yet flexible object-oriented programming and graphical interfaces have been largely instrumental in enabling the practical use of these resource-and-data-intensive systems. There is demonstrated great potential for enhanced practical use of planning and scheduling systems that can benefit from the joint employment of machine learning-based analytics (such as artificial neural networks or data mining with decision trees) and artificial intelligence-based cognitive techniques (such as expert systems) coupled with the latest clever mathematical algorithms made possible by high-performance computer hardware (as also mentioned elsewhere). In view of current developments, model-based computer systems are increasingly if not pervasively substituting the function of many manual (nonautomated) procedures, which typically rely on spreadsheet-based tools presently used for planning and scheduling activities of complex refineries (particularly in handling multiple crude oils processing). These activities frequently entail making decisions for multiperiod problems that involve optimization to sequence crude oil runs with consideration for product blending rules, allocate storage and charging tanks, determine operating conditions of the process units and their associated auxiliary or supporting units, devise product blending formulations, and sequence the movements of finished products for distribution to depots or ports as well as to be ready for shipping to sales points of end customers.

#### 1.3.5.1 Systems Implementation

Planning and scheduling systems are at the heart of refinery IT systems as well as increasingly its OT systems. Thus it is imperative that data for the plans and schedules are continuously kept up to date. The main data required comprises tank levels (as a function of time) especially those related to inventory, operating conditions of process units, component and product qualities, and major equipment availability besides business-related data such as marketing requirements (or situations) as well as forecast of external supply or deliveries and product lifting requirements.

Refineries require robust, reliable, and secure communications network that include auxiliary systems such as an associated database to store plant-wide data for the necessary or requisite processing and manipulation steps of extraction, transformation, and loading to the relevant applications. This infrastructure is deemed as crucial elements or components yet with potential room for major improvements particularly in view of harnessing the pervasive "big data" available today in deriving greater value from better decision-making activities. Planning and scheduling functions are now adopted as decision support systems. However the scope of such systems typically do not guarantee whole refinery optimization of the operations, mainly due to the challenge of high complexity and consequently a long model solution time (i.e. runtime).

It is typically practiced in the industry to develop separate modeling applications on crude oil charging and blend scheduling (at refinery front-end) and that on planning and scheduling of product blending and delivery (at refinery back-end). Plans and schedules tend to be obsolete (i.e. no longer relevant to business situations) fairly rapidly due to uncertain product demands and other market-related factors or even sentiments. For the latter problem, the uncertainty arising from fluctuating product demands and other changing parameters of the market often render the plans and especially the schedules to be obsolete very quickly. Thus, such problems (particularly the schedules) are mainly used for optimization studies on the products tankage.

#### 1.3.5.2 Optimization of Crude Oil Scheduling

As crude oil purchasing costs account for more than two-thirds (around 80%) of a refinery's turnover, we can achieve significant savings by optimally performing the scheduling operation of charging crude oil blends to the primary (atmospheric) distillation units (Kelly and Mann 2003). With premium crude oils experiencing reduced supplies and increased prices or costs, a significant operational optimization issue that afflicts refineries today revolves around how to feasibly (if not optimally) exploit greater margins from employing low-cost crude oils or the so-called "challenged crudes", i.e. to increase profits by using varying blends of premium and challenged crude oils. However, various operational issues are expected to arise related to processing these challenged crudes that have high contents of contaminants including aromatics, sulfur, and various other high residues. Therefore, refiners need to strategically identify an optimal mix of both premium and challenged crude oils for processing that does not compromise profit margins and with as few operational challenges as possible to this crude oil blend scheduling optimization problem.

It is not surprising that the functions, duties, and responsibilities of refinery crude oil schedulers (i.e. optimization application users) are not only ever more demanding and pressing now but increasingly complex and convoluted, which entails increasingly higher risks at stake operationally, financially, and politically. It is requisite that the users monitor and match crude oil movement to market demand as well as that of the refinery overall operation.

Under normal circumstances of handling crude oil receipts or arrivals, the users assign destination tanks for each of the crude oil shipment parcels. This task also includes blending and charging the received crude oils to the distillation units (i.e. CDU) as necessary in meeting mainly yield and quality targets or various other specifications on the fractionation products. However, due to pressures arising from timing or deadlines and unfavorable inventory availability or flexibility, the users tend to rely on their experience (if not intuition) that prompts them to select the first feasible solution computed by existing non-rigorous model-based tools (e.g. spreadsheets using Excel typically). As a result, there is significant loss of economic and operational opportunities to improve such planning and scheduling decision-making activities.

Automated, reliable, and robust model-based refinery crude oil blend scheduling optimization system is valuable and needed for the foregoing reasons with potential of enhancing crude oil blend options by considering various possible (and permissible) charge mixtures (i.e. combinations or permutations of crude oil sources or types in optimum proportions) particularly in capturing value from processing high-quality crude oils which are mixed with less expensive feedstock in an economically optimum manner. Other associated benefits or returns that such advanced optimization systems can offer include increased throughput (i.e. processing output) and raw material resource utilization, reduced yield and quality giveaways, enhanced control and predictability of downstream production, and decreased costs (e.g. inventory holding, storage, and demurrage).

#### 1.3.5.3 Refinery Management

A real challenge in using modeling tools lies in ensuring that we can get realistic results compared to an existing possibly manual approach. With the present drive for harnessing the power and resultant benefit of increased digitalization, it is imperative to be able to showcase and continually improve the value of modeling (or a model-driven approach, in general) to refiners. The outcome of improvement brought about through such efforts typically requires minimal additional bespoke or tailored custom-built features with a potential incentive that they can be directly adopted to meet actual refinery operations while the derived benefits can be straightforwardly quantified (e.g. in monetary sense). Some of the advancements include linking model-based optimization tools with real-time databases for which such automation permits access to data and insights that could assist with planning and scheduling activities. An example entails validating outputs from (long-term) plans and (short-term) schedules enhanced with simulation results with an aim of gaining more granularity toward attaining more realistic production targets setting.

## 1.4 Concluding Remarks

This chapter provides an overview of the subject addressed in this book, which concerns a mixed-integer superstructure optimization approach to determine the topology or configuration for a petroleum refinery. A brief treatment of refining processes is given as background on the numerous available commercial process units considered in the approach. The chapter then proceeds to present a representative selection of staple refinery optimization modeling tools as partly exemplified by the current practice of RTO and APC. A brief exposition is also offered as regards to modeling-aided suite of techniques and approaches for efficient and effective plant management as appropriate in this age of digitalization as spurred by Industrial Revolution 4.0, big data analytics, and to a certain extent, the global coronavirus (Covid-19) outbreak, chiefly to lend a flavor to the book's subject but without attempting to be comprehensive (with references cited for a more complete exposition).

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