1.3 WHAT IS PROCESS SYNTHESIS?

Synthesis involves putting together separate elements into a connected or a coherent whole. The term "process synthesis" dates back to the early 1970s and gained much attention with the seminal book of Rudd et al. (1973). Process synthesis may be defined as (Westerberg 1987): "the discrete decision-making activities of conjecturing (1) which of the many available component parts one should use, and (2) how they should be interconnected to structure the optimal solution to a given design problem". Process synthesis is concerned with the activities in which the various process elements are combined and the flowsheet of the system is generated so as to meet certain objectives. Therefore, the aim of process synthesis (Johns 2001) is: "to optimize the logical structure of a chemical process, specifically the sequence of steps (reaction, distillation, extraction, etc.), the choice of chemical employed (including extraction agents), and the source and destination of recycle streams". Hence, in process synthesis we know process inputs and outputs and are required to revise the structure and parameters of the flowsheet (for retrofitting design of an existing plant) or create a new flowsheet (for grassroot design of a new plant). This is shown in Figure 1-2.

Reviews on process synthesis techniques are available in literature (e.g., Westerberg 2004; Seider et al., 2003; Biegler et al., 1997; Smith 1995; Stephanopoulos and Townsend 1986).

The result of process synthesis is a flowsheet which represents the configuration of the various pieces of equipment and their interconnection. Next, it is necessary to analyze the performance of this flowsheet.

1.4 WHAT IS PROCESS ANALYSIS?

While synthesis is aimed at combining the process elements into a coherent whole, analysis involves the decomposition of the whole into its constituent elements for individual study of performance. Hence, process analysis can be contrasted (and complemented) with process synthesis. Once an alternative is generated or a process is synthesized, its detailed characteristics (e.g., flowrates, compositions, temperature, and pressure) are predicted using analysis techniques. These techniques include mathematical models, empirical correlations, and computer-aided process simulation tools. In addition, process analysis may involve predicting and validating performance using

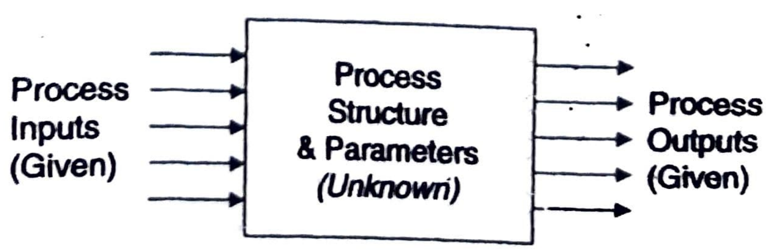

FIGURE 1-2 PROCESS SYNTHESIS PROBLEMS

experiments at the lab and pilot-plant scales, and even actual runs of existing facilities. Thus, in *process analysis* problems we know the process inputs along with the process structure and parameters while we seek to determine the process outputs (Figure 1-3).

1.5 WHY INTEGRATION?

Now, we turn our attention to a motivating example on coal pyrolysis process. A simplified flowsheet of the process is shown in Figure 1-4. The main products are different hydrocarbon cuts. Benzene is further processed in a dehydrogenation reactor to produce cyclohexane. A hydrogen-rich gas is produced out of the cyclohexane reactor and is currently flared. Medium and heavy distillates contain objectionable materials (primarily sulfur, but

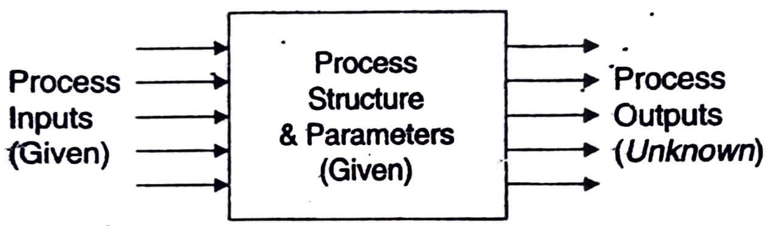

FIGURE 1-3 PROCESS ANALYSIS PROBLEM

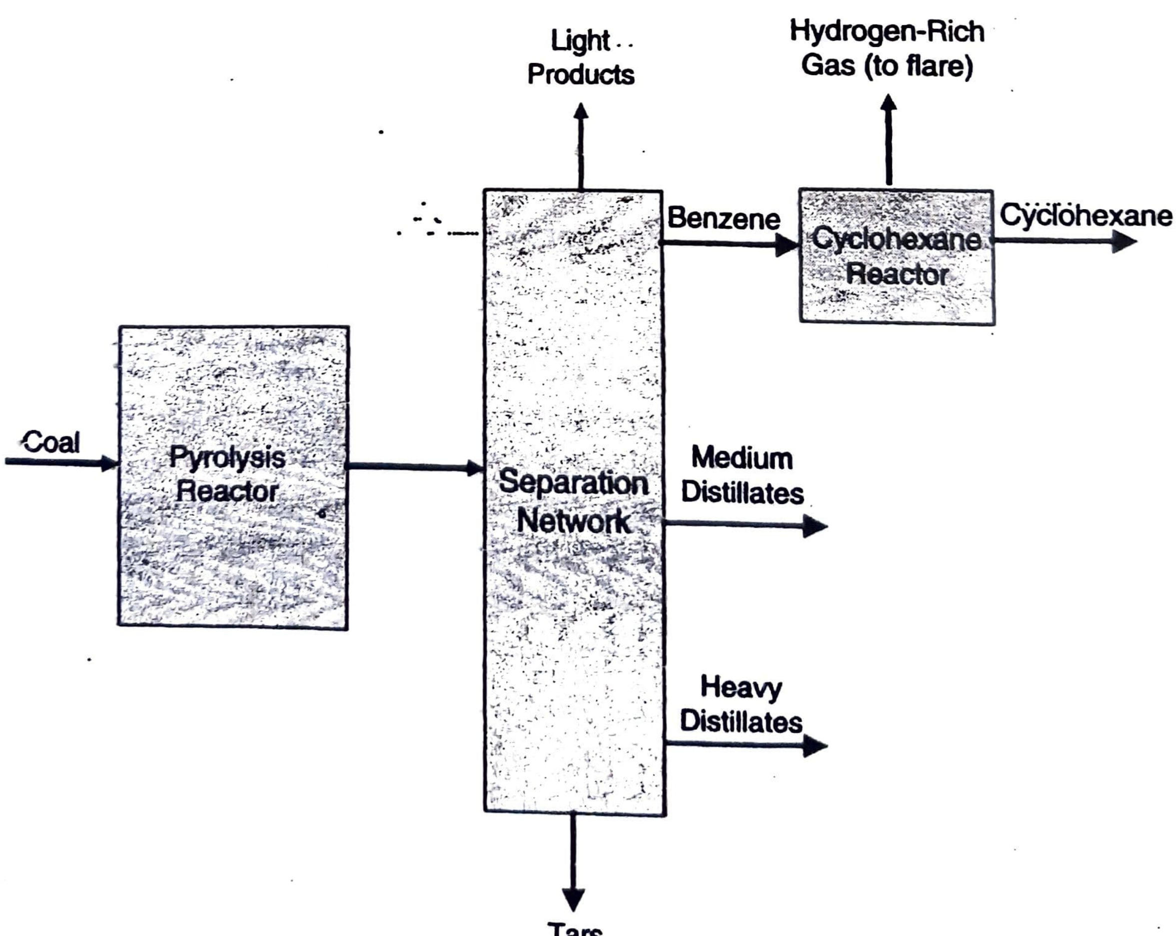

FIGURE 1-4 PYROLYSIS OF COAL

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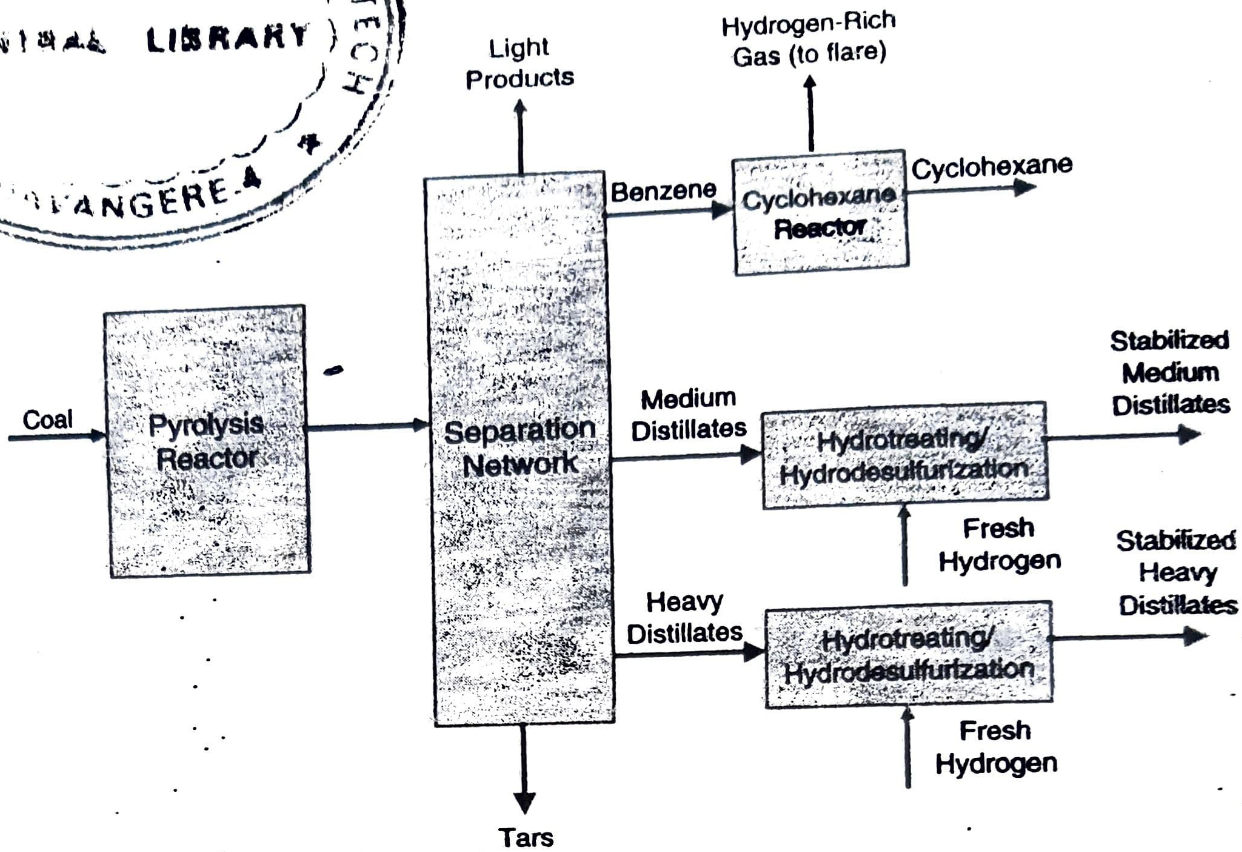

FIGURE 1-5 SYNTHESIZED FLOWSHEET FOR STABILIZATION OF MEDIUM AND HEAVY DISTILLATES

also nitrogen, oxygen, halides) that should be removed and unsaturated hydrocarbons (e.g. olefins and gum-forming unstable diolefins) that should be converted to paraffins. Our design objective is to synthesize a revised process to remove sulfur (and other objectionable materials) and stabilize olefins and diolefins. One way of addressing the problem is to synthesize a revised flowsheet that include hydrotreating and hydrodesulfurization units as shown in Figure 1-5. These units employ fresh hydrogen to remove the objectionable materials and stabilize the olefins and diolefins. This is a synthesized solution that will work, but what is wrong with this solution? There is *no integration* of mass (hydrogen). On one hand, fresh hydrogen is purchased and used in hydrotreating/hydrodesulfurization. On the other hand, hydrogen produced from benzene dehydrogenation is flared. Integration of mass is needed to conserve resources and reduce cost.

Reflecting back on the AN case study, the original flowsheet (Figure 1-1a) suffered from lack of water integration. While fresh water was used in the boiler and the scrubber, wastewater was discharged into biotreatment. The various alternatives to solve the AN example attempted to provide some level of water integration.

Next, let us consider the pharmaceutical processing facility (El-Halwagi 1997) illustrated in Figure 1-6. The feed mixture (C_1) is first heated to 550 K, then fed to an adiabatic reactor where an endothermic reaction takes place. The off-gases leaving the reactor (H_1) at 520 K are cooled to 330 K prior to being forwarded to the recovery unit. The mixture leaving the bottom of the reactor is separated into a vapor fraction and a slurry fraction.

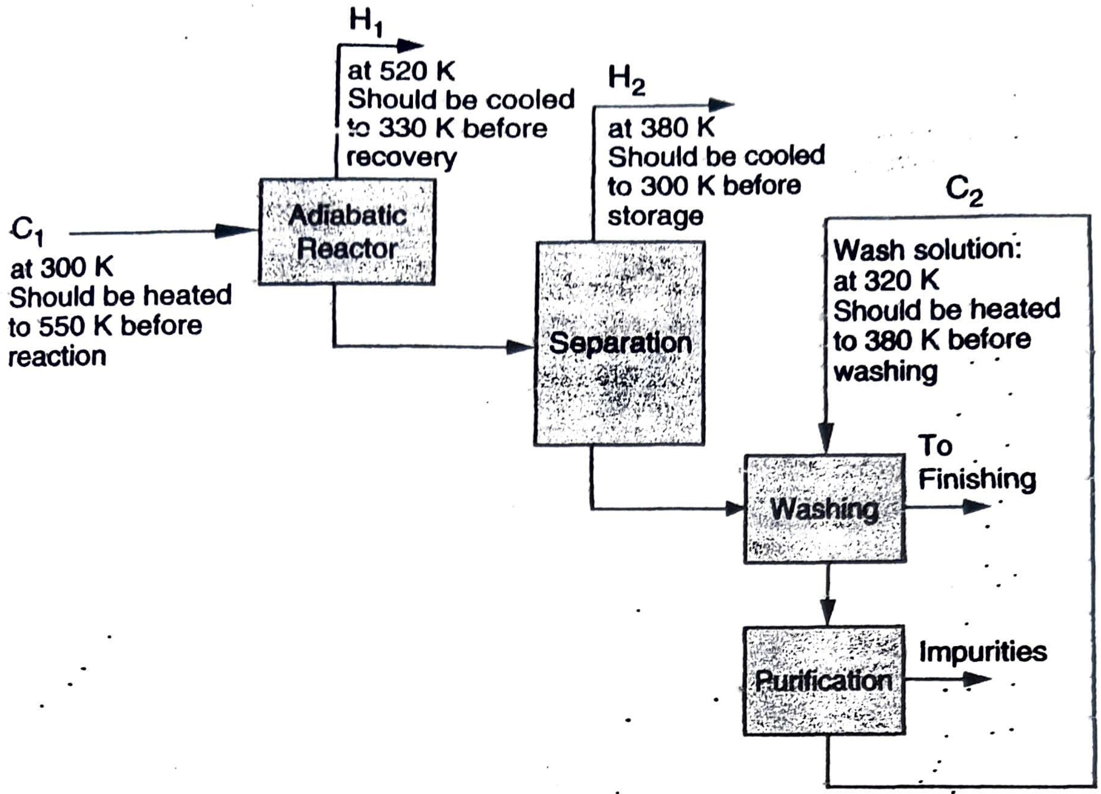

FIGURE 1-6 HEATING AND COOLING REQUIREMENTS FOR PHARMACEUTICAL PROCESS (EL-HALWAGI 1997)

The vapor fraction (H_2) exits the separation unit at 380 K and is to be cooled to 300 prior to storage. The slurry fraction is washed with a hot immiscible liquid at 380 K. The wash liquid is purified and recycled to the washing unit. During purification, the temperature drops to 320 K. Therefore, the recycled liquid (C_2) is heated to 380 K.

One alternative for synthesizing a solution that addresses the energy requirements for the pharmaceutical process is to add two heaters and two coolers that respectively employ a heating utility (e.g., steam, heating oil) and a cooling utility (e.g., cooling water, refrigerant). This solution (Figure 1-7) will work, but what is wrong with it? There is *no integration of heat*. There are two process hot streams to be cooled and two process cold streams to be heated. It seems advantageous to attempt to transfer heat from the process hot streams to the process cold streams before paying for external heating and cooling utilities. In fact, exchanging heat between process hot streams and process cold streams will result in a simultaneous reduction in the usage of external heating and cooling utilities. In addition to cost savings, the process will also conserve natural resources by virtue of decreasing the consumption of fuel and other energy sources needed for the generation of heating and cooling utilities.

The foregoing discussion highlights the need for an integration framework to guide and assist process synthesis activities and conserve process resources. This is the scope of process integration.

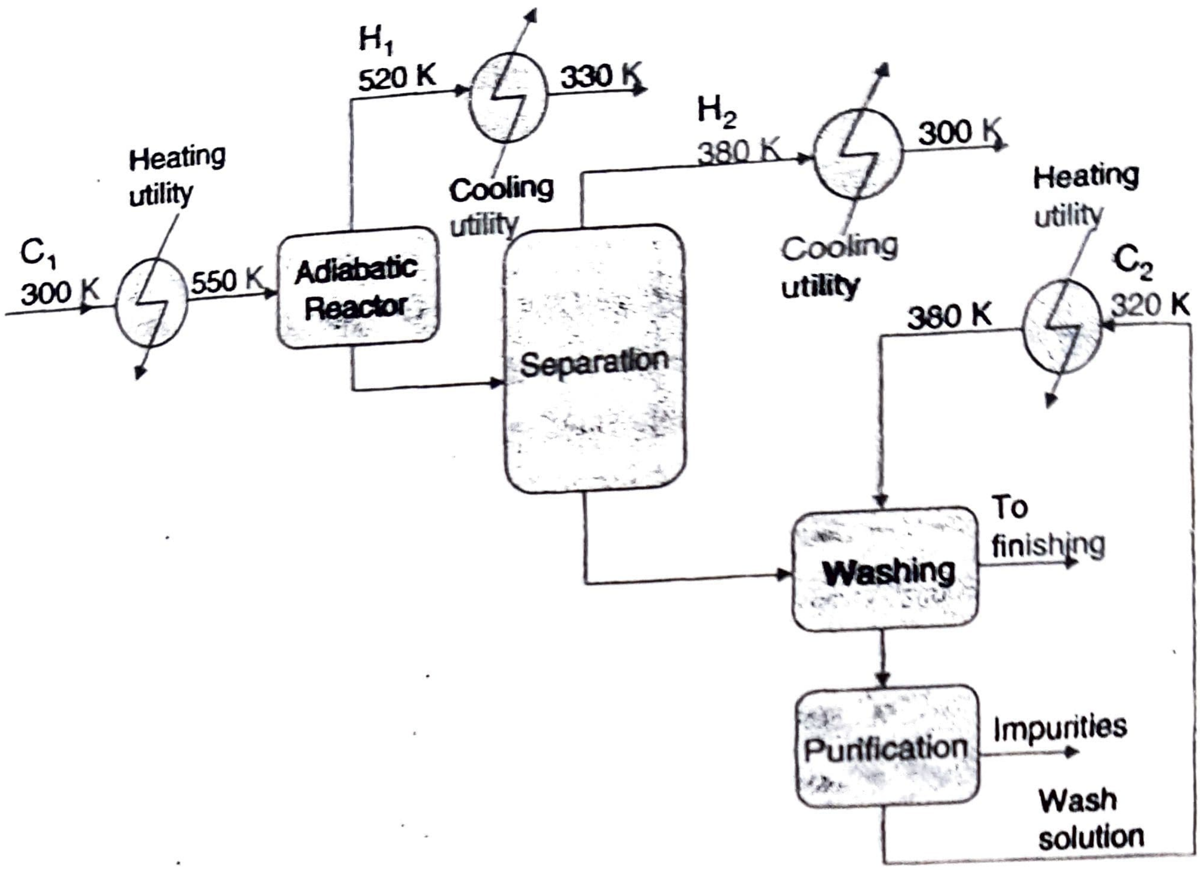

FIGURE 1-7 HEATING AND COOLING REQUIREMENTS FOR PHARMACEUTICAL PROCESS (EL-HALWAGI 1997)

1.6 WHAT IS PROCESS INTEGRATION?

A chemical process is an integrated system of interconnected units and streams. Proper understanding and solution of process problems should not be limited to symptoms of the problems but should identify the root causes of these problems by treating the process as a whole. Furthermore, effective improvement and synthesis of the process must account for this integrated nature. Therefore, integration of process resources is a critical element in designing and operating cost-effective and sustainable processes. *Process integration is a holistic approach to process design, retrofitting, and operation which emphasizes the unity of the process* (El-Halwagi 1997). In light of the strong interaction among process units, resources, streams, and objectives, process integration offers a unique framework for fundamentally understanding the global insights of the process, methodically determining its attainable performance targets, and systematically making decisions leading to the realization of these targets.

Process integration involves the following activities:

1. Task Identification: The first step in synthesis is to explicitly express the goal we are aiming to achieve and describe it as an *actionable* task. The actionable task should be defined in such a way so as to capture the essence of the original goal. For instance, quality enhancement may be described as a task to reach a specific

composition or certain properties of a product. Another example is in the AN case study, the debottlenecking objective may be expressed as a wastewater-reduction task which entails water integration. In the case of the coal pyrolysis example, the task of stabilizing the middle and heavy distillates can be expressed as a hydrodesulfurization/hydrotreating task which involves hydrogen integration. In characterizing the task, we should describe the salient information and constraints. Additionally, the task should be characterized by some quantifiable metrics. For instance, the task may be quantified with an extreme performance (e.g., minimum wastewater discharge), a specific value (e.g., 50% reduction in wastewater), or as a multivariable function (e.g., relationship between extent of wastewater reduction and pollutant content).

2. Targeting: The concept of targeting is one of the most powerful contributions of process integration. *Targeting refers to the identification of performance benchmarks ahead of detailed design.* In a way, you can find the ultimate answer without having to specify how it may be reached! For instance, in the AN example what is the target for minimum wastewater discharge. As shown in Chapter Five, this target is 4.8 kg/s and it can be determined without discussing how it can be reached. Similarly, in the pharmaceutical process, the targets for minimum heating and cooling utility requirements are 2620 and 50 kW, respectively. Again, these targets can be rigorously determined without conjecturing how the implementation of the heat-integration scheme looks like. Targeting allows us to determine how far we can push the process performance and sheds useful insights on the exact potential and realizable opportunities for the process. Even if we elect not to reach the target, it is still useful to benchmark current performance versus the ultimate performance.
3. Generation of Alternatives (Synthesis): Given the enormous number of possible solutions to reach the target (or the defined task), it is necessary to use a framework that is rich enough to embed all configurations of interest and represent alternatives that aid in answering questions such as: How should streams be rerouted? What are the needed transformations (e.g., separation, reaction, heating, etc.)? For example, should we use separations to clean up wastewater for reuse? To remove what? How much? From which streams? What technologies should be employed? For instance, should we use extraction, stripping, ion exchange, or a combination? Where should they be used? Which solvents? What type of columns? Should we change operating conditions of some units? Which units and which operating conditions? The right level of representation for generating alternatives is critically needed to set capture the appropriate design space. Westerberg (2004) underscores this point by stating that "It is crucial to get the representation right. The right representation can enhance insights. It can aid innovation".

4. Selection of Alternative(s) (Synthesis): Once the search space has been generated to embed the appropriate alternatives, it is necessary to extract the optimum solution from among the possible alternatives. This step is typically guided by some performance metrics that assist in ranking and selecting the optimum alternative. Graphical, algebraic, and mathematical optimization techniques may be used to select the optimum alternative(s). It is worth noting that the generation and selection of alternatives are *process synthesis* activities.
5. Analysis of Selected Alternative(s): Process analysis techniques can be employed to evaluate the selected alternative. This evaluation may include prediction of performance, techno-economic assessment, safety review, environmental impact assessment, etc.

It is instructive to reiterate the difference between targeting and the generation/selection of alternatives. Targeting is a structure-independent approach while the generation and selection of alternative configurations is structure based (El-Halwagi and Spriggs 1998; El-Halwagi 1997). The structure-independent (or targeting) approach is based on tackling the task via a sequence of stages. Within each stage, a design target can be identified and employed in subsequent stages. Such targets are determined ahead of detailed design and without commitment to the final system configuration. The targeting approach offers two main advantages. First, within each stage, the problem dimensionality is reduced to a manageable size, avoiding the combinatorial problems. Second, this approach offers valuable insights into the system performance and characteristics.

The structure-dependent approach to the generation and selection of alternatives involves the development of a framework that embeds all potential configurations of interest. Examples of these frameworks include process graphs (e.g. Brendel et al., 2000; Kovacs et al., 2000; Friedler et al., 1995), state-space representation (e.g., Martin and Manousiouthakis 2001; Bagajewicz and Manousiouthakis 1992), and superstructures (e.g., Biegler et al., 1997; Floudas et al., 1986). The mathematical representation used in this approach is typically in the form of mixed-integer non-linear programs (MINLPs). The objective of these programs is to identify two types of variables; integer and continuous. The integer variables correspond to the existence or absence of certain technologies and pieces of equipment in the solution. For instance, a binary integer variable can assume a value of one when a unit is selected and zero when it is not chosen as part of the solution. On the other hand, the continuous variables determine the optimal values of nondiscrete design and operating parameters such as flowrates, temperatures, pressures, and unit sizes. Although this approach is potentially more robust than the structure-independent strategies, its success depends strongly on three challenging factors. First, the system representation should embed as many potential alternatives as possible. Failure to incorporate certain configurations may result in suboptimal solutions. Second, the non-linearity properties of the composition or certain properties of a product. Another example is in the AN case study, the debottlenecking objective may be expressed as a wastewater-reduction task which entails water integration. In the case of the coal pyrolysis example, the task of stabilizing the middle and heavy distillates can be expressed as a hydrodesulfurization/hydrotreating task which involves hydrogen integration. In characterizing the task, we should describe the salient information and constraints. Additionally, the task should be characterized by some quantifiable metrics. For instance, the task may be quantified with an extreme performance (e.g., minimum wastewater discharge), a specific value (e.g., 50% reduction in wastewater), or as a multivariable function (e.g., relationship between extent of wastewater reduction and pollutant content).

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1.7 CATEGORIES OF PROCESS INTEGRATION

Over the past two decades, numerous contributions have been made in the field of process integration. These contributions may be classified in different ways. One method of classification is based on the two main commodities consumed and processed in a typical facility: energy and mass. Therefore, from the perspective of resource integration, process integration may be classified into energy integration and mass integration. *Energy integration* is a systematic methodology that provides a fundamental understanding of energy utilization within the process and employs this understanding in identifying energy targets and optimizing heat-recovery and energy-utility systems. On the other hand, *mass integration* is a systematic methodology that provides a fundamental understanding of the global flow of mass within the process and employs this understanding in identifying performance targets and optimizing the generation and routing of species throughout the process. The fundamentals and applications of energy and mass integration have been reviewed in literature (e.g., Rossiter 2004; Dunn and El-Halwagi 2003; Hallale 2001; Smith 2000; El-Halwagi and Spriggs 1998; El-Halwagi 1997; Shenoy 1995; Linnhoff 1994; Gundersen and Naess 1988; Douglas 1988). More recently, a new category of process integration has been introduced. It is referred to as "property integration". Chapter Eight provides on overview of property integration and how it can be used to optimize the process and conserve resources by tracking properties and functionalities.

1.8 STRUCTURE OF THE BOOK

This book presents the fundamentals and applications of process integration. Holistic approaches, methodical techniques, and step-by-step procedures are presented and illustrated by a wide variety of case studies. Visualization, algebraic, and mathematical programming techniques are used to explain and address process integration problems. The first five chapters of the book focus on graphical approaches. Chapters six and seven illustrate the use of algebraic tools. The rest of the book introduces mathematical programming techniques in conjunction with graphical and algebraic methods. The covered topics include mass integration, energy integration, and property integration. The scope of problems ranges from identification of overall performance targets to integration of separation systems, recycle networks, and heat exchange networks. Numerous case studies are used