# CHAPTER ONE

# INTRODUCTION TO PROCESS INTEGRATION

The process industries are among the most important manufacturing facilities. They span a wide range of industries including chemical, petroleum, gas, petrochemical, pharmaceutical, food, microelectronics, metal, textile, and forestry products. The performance of these industries is strongly dependent on their engineering and engineers. So, what are the primary responsibilities of process engineers in the process industries? Many process engineers would indicate that their role in the process industries is to design and operate industrial processes and make them work faster, better, cheaper, safer, and greener. All of these tasks lead to more competitive processes with desirable profit margins and market share. Specifically, these responsibilities may be expressed through the following specific objectives:

- Process innovation
- Profitability enhancement
- Yield improvement
- Capital-productivity increase
- Quality control, assurance, and enhancement
- Resource conservation
- Pollution prevention
- Safety
- Debottlenecking

These objectives are also closely related to the seven themes identified by Keller and Bryan (2000) as the key drivers for process-engineering research, development, and changes in the primary chemical process industries. These themes are:

- Reduction in raw-material cost
- Reduction in capital investment

- Reduction in energy use
- Increase in process flexibility and reduction in inventory
- Ever greater emphasis on process safety
- Increased attention to quality
- Better environmental performance

The question is how? What are the challenges, required methodologies, and enabling tools needed by engineers to carry out their responsibilities? In order to shed some light on these issues, let us consider the following motivating example.

## 1.1. GENERATING ALTERNATVIES FOR DEBOTTLENECKING AND WATER REDUCTION IN ACRYONITRILE PROCESS

Consider the process shown in Fig. 1a for the production of acrylonitrile $(AN,\ C_3H_3N)$. The main reaction in the process involves the vapor phase catalytic reaction of propylene, ammonia, and oxygen at 450$^{o}$C and 2 atm. To produce AN and water, i.e.

$$C_3H_6+NH_3+1.5O_2\xrightarrow{catalyst}C_3H_3N+3H_2O.$$

The reaction products are quenched in an indirect-contact cooler/condenser which condenses a portion of the reactor off-gas. The remaining off-gas is scrubbed with water, then decanted into an aqueous layer and an organic layer. The organic layer is fractionated in a distillation column under slight vacuum which is induced by a steam-jet ejector. Wastewater is collected from from four process streams: off-gas condensate, aqueous layer of decanter, distillation bottoms, and jet-ejector condensate. The wastewater stream is fed to the biotreatment facility. At present, the biotreatment facility is operating at full hydraulic capacity and, consequently, it constitutes a bottleneck for the plant. The plant has a sold-out profitable product and wishes to expand. Our task is debottleneck the process.

The intuitive response to debottlenecking the process is to construct an expansion to the biotreatment facility (or install another one). This solution focuses on the symptom of the problem: the biotreatment is filling up, therefore we must its expand capacity. A legitimate question is whether there are other solutions, probably superior ones, that will address the problem by making in-plant process modifications as opposed to “end-of-pipe“ solution? Invariably, the answer in this case and most other process design problems is “yes”. If so, how do we determine the root causes of the problem (not just the symptoms) and how can we generate superior solutions? Where do we start and how do address the problem?

For now, let us start with a conventional engineering approach involving a brainstorming session among a group of process engineers who will generate a number of ideas and evaluate them. Since the objective is to debottleneck the biotreatment facility, then an effective approach may be based on reducing the influent wastewater flowrate into biotreatment. One way of reducing wastewater flowrate is to adopt a wastewater recycle strategy in which it is desired to recycle some (or all) of the wastewater to the process. For instance, let us recycle some of the wastewater to the distillation column (Fig. 1b). After analyzing this solution, it does not seem to be effective. The fresh water to the process is still the same, water generated by the main AN-producing reaction is the same, and therefore the wastewater leaving the plant will remain the same. So, let us employ a recycle strategy that replaces fresh water with wastewater. This way, the fresh water into the process is reduced and, consequently, the wastewater leaving the process will be reduced as well. One option is to recycle the wastewater to the scrubber (Fig. 1c) assuming that it is feasible to process the wastewater in the scrubber without negatively impacting the process performance. In such cases, both fresh water and wastewater will be reduced. Alternatively, it may be possible to recycle the wastewater to the boiler (Fig. 1d). Along the same lines, the wastewater may be recycled to both the scrubber and the boiler (Fig. 1e). However, how should the wastewater be distributed between the two units? One can foresee many possibilities for distribution (50-50, 51-49, 60-40, 99-1, etc.). Another alternative is to consider segregating (avoiding the mixing of) the wastewater streams. Segregation would prevent some wastewater streams from mixing with the more polluted streams, thereby enhancing their likelihood for recycle. For instance, the off-gas condensate and the decanter aqueous layer may be segregated from the two other wastewater streams and recycled to the scrubber and the boiler (Fig. 1f). Clearly, there are many alternatives for segregation and recycle. In order to safeguard against the accumulation of impurities or the detrimental effects of replacing fresh water with waste streams, it may be necessary to consider the use of separation technologies to clean up the streams and render them in a condition acceptable for recycle. For example, a separator may be installed to treat the decanter wastewater (Fig. 1g). But, what separation technologies should be used? To remove what? From which streams? Figures 1g – 1i are just three possibilities (out of numerous alternatives) for the type and allocation of separation technologies. And so on! Clearly, there are ***infinite number of alternatives*** that can solve this problem. So many decisions have to be made on the rerouting of streams, the distribution of streams, the changes to be made in the process (including design and operating variables), the substitution of materials and reaction pathways, and the replacement or addition of units. It is worth describing the optimum solution (in terms of cost) to this problem as shown in Fig. 1j. The development of this solution will be shown in details in Chapter Five.

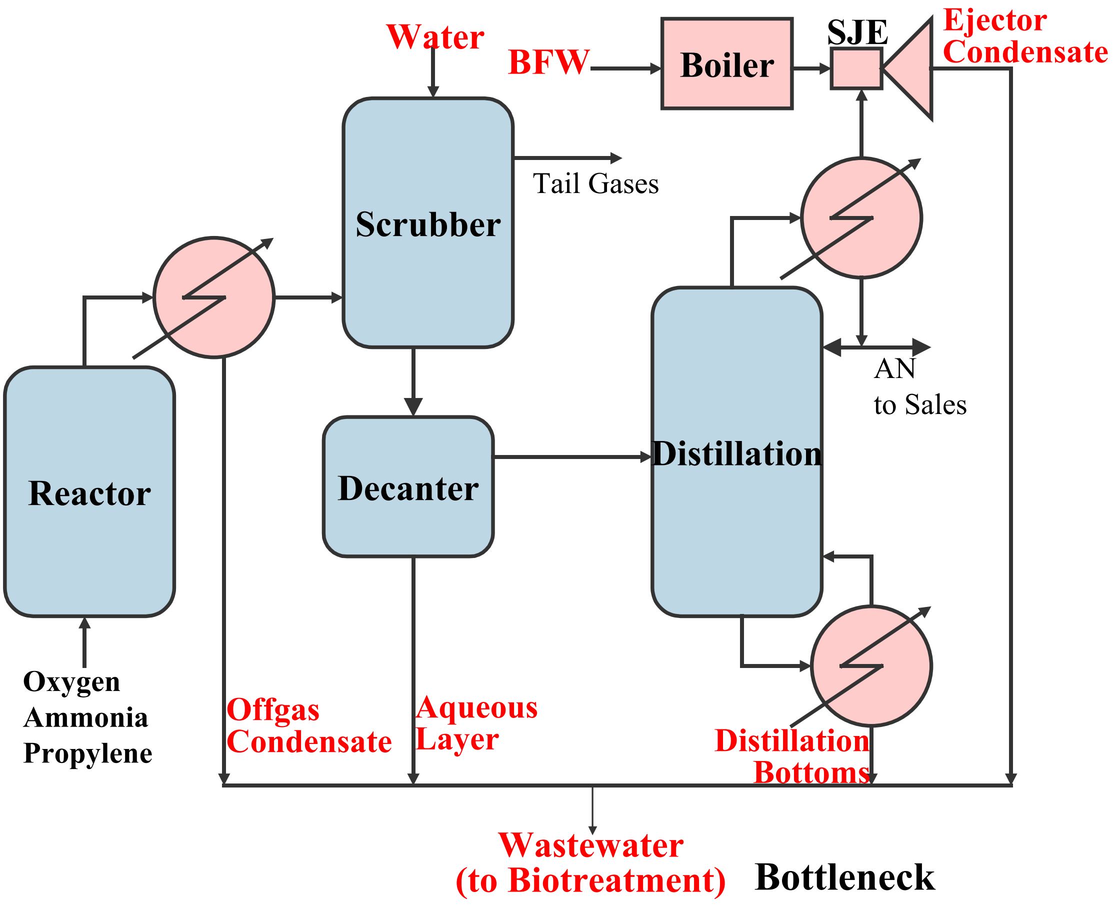

Fig. 1a. Process for AN Manufacture (El-Halwagi, 1997)

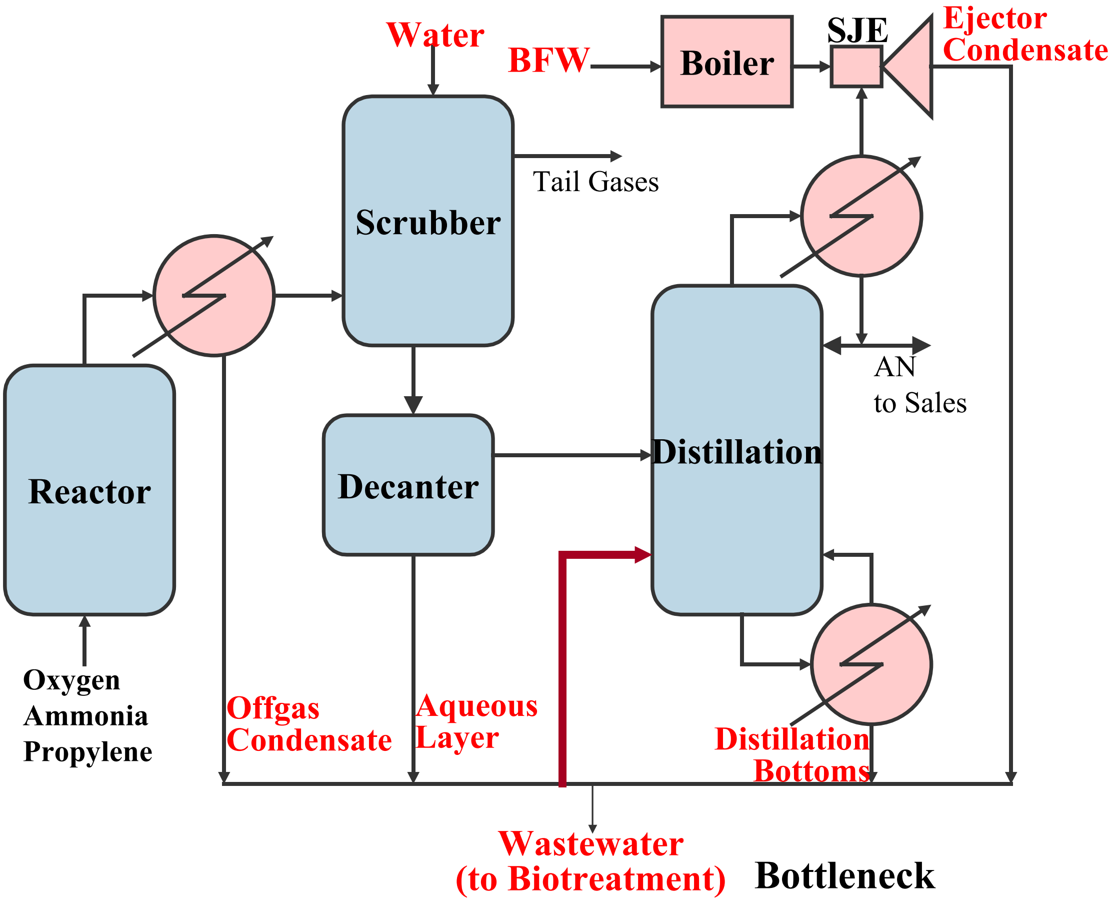

Fig. 1b. Recycle to the Distillation Column

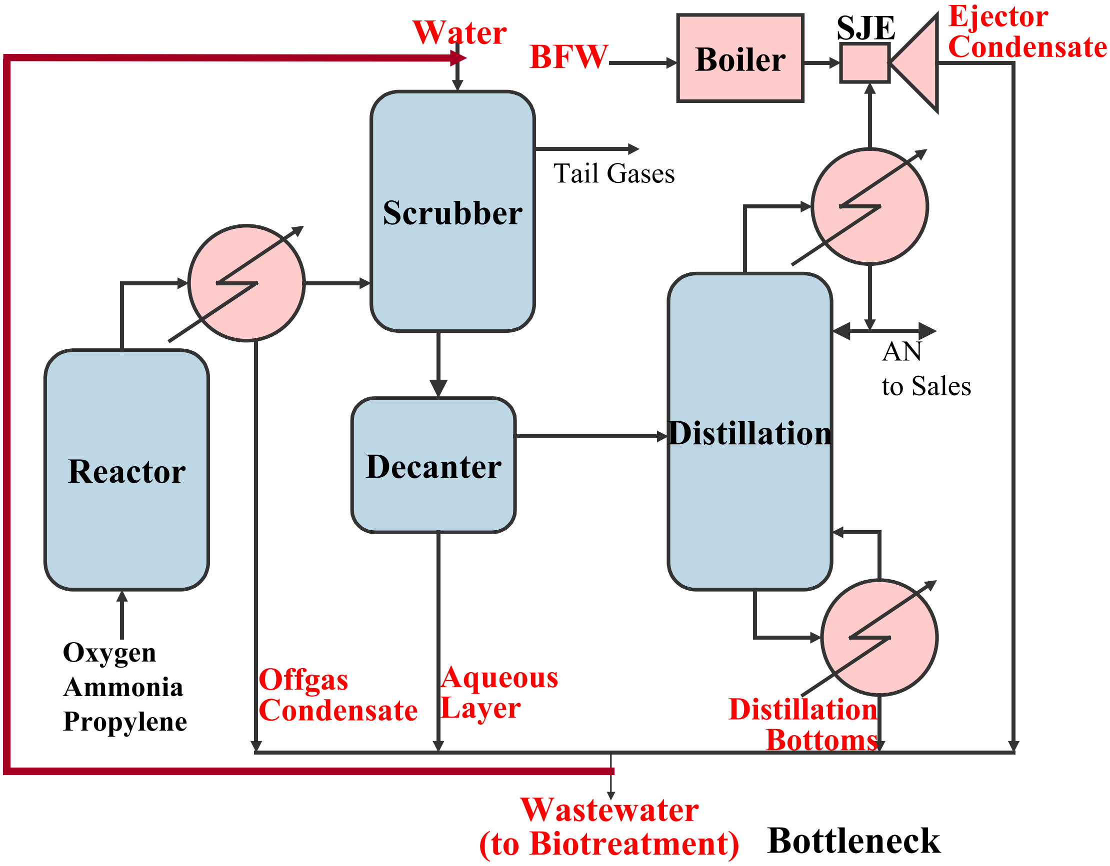

Fig. 1c. Recycle to Replace Scrubber Water

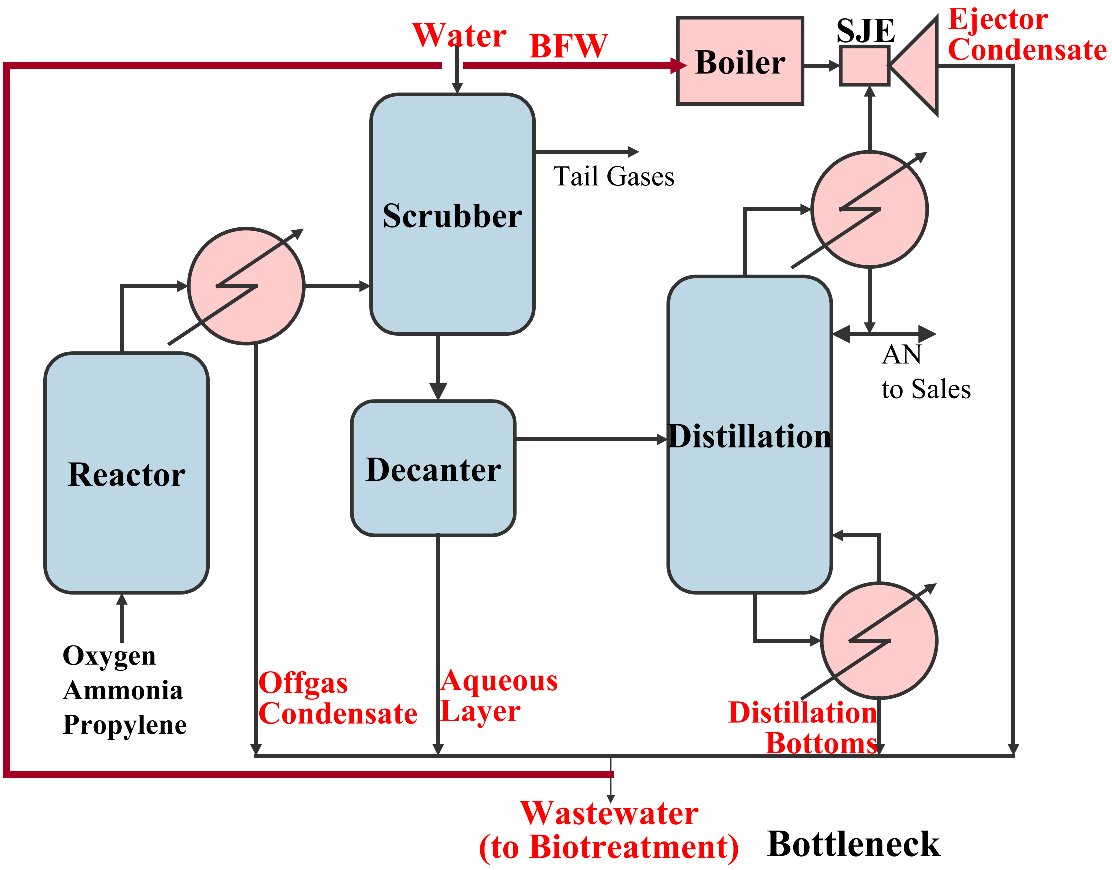

Fig. 1d. Recycle to Substitute Boiler Feed Water

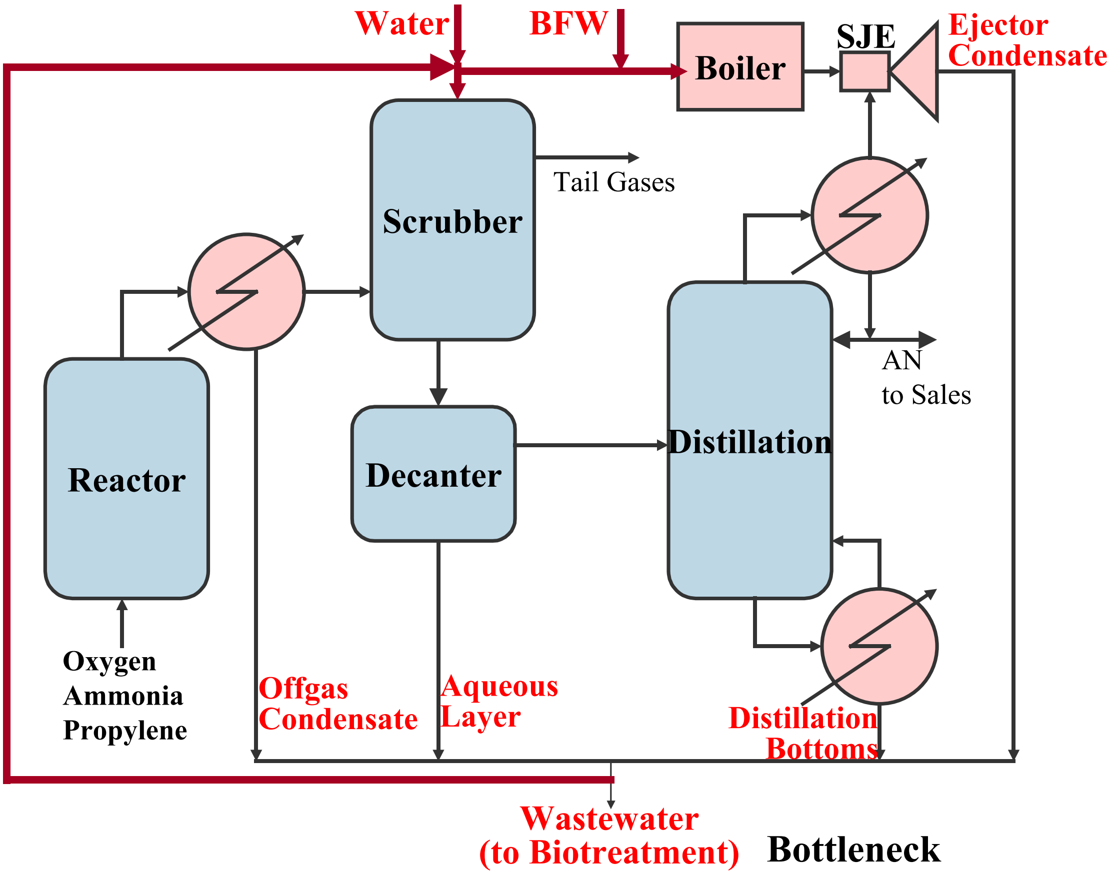

Fig. 1e. Recycle to Both Scrubber and Boiler

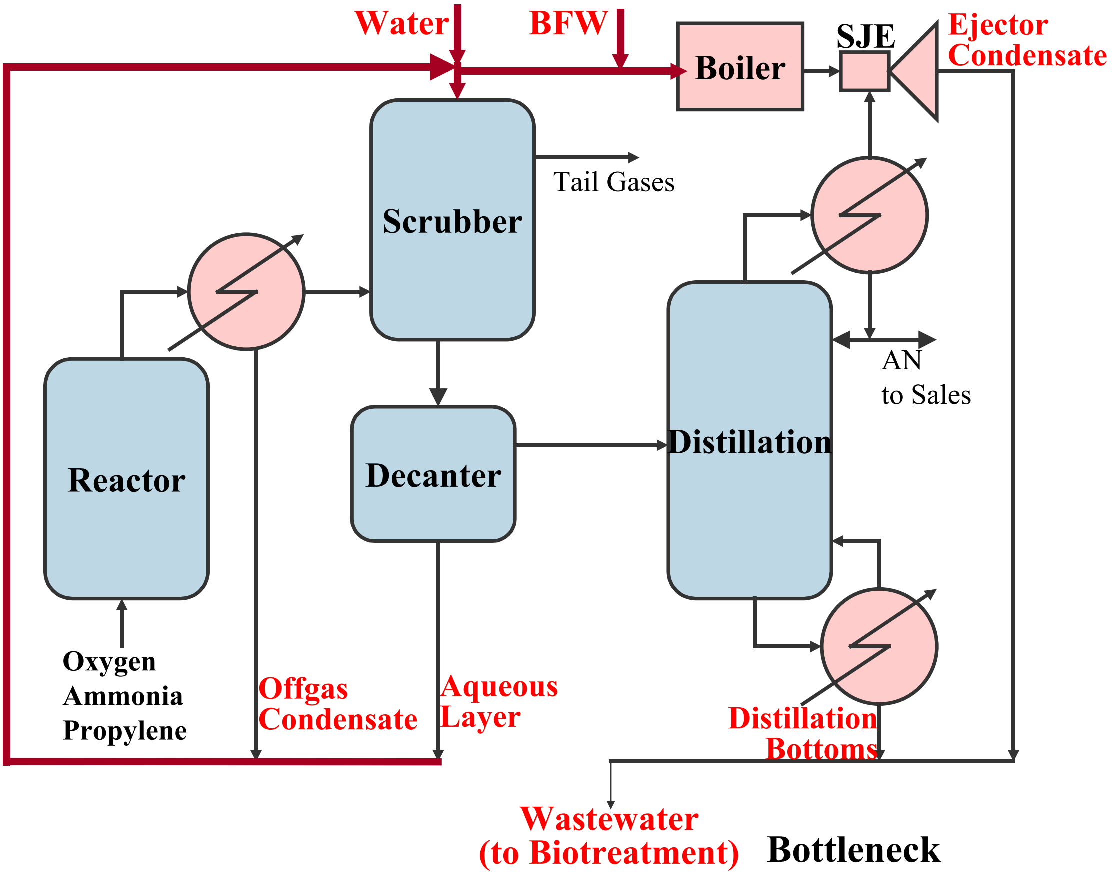

Fig. 1f. Segregation of Wastewater and Recycle of Two Segregated Streams

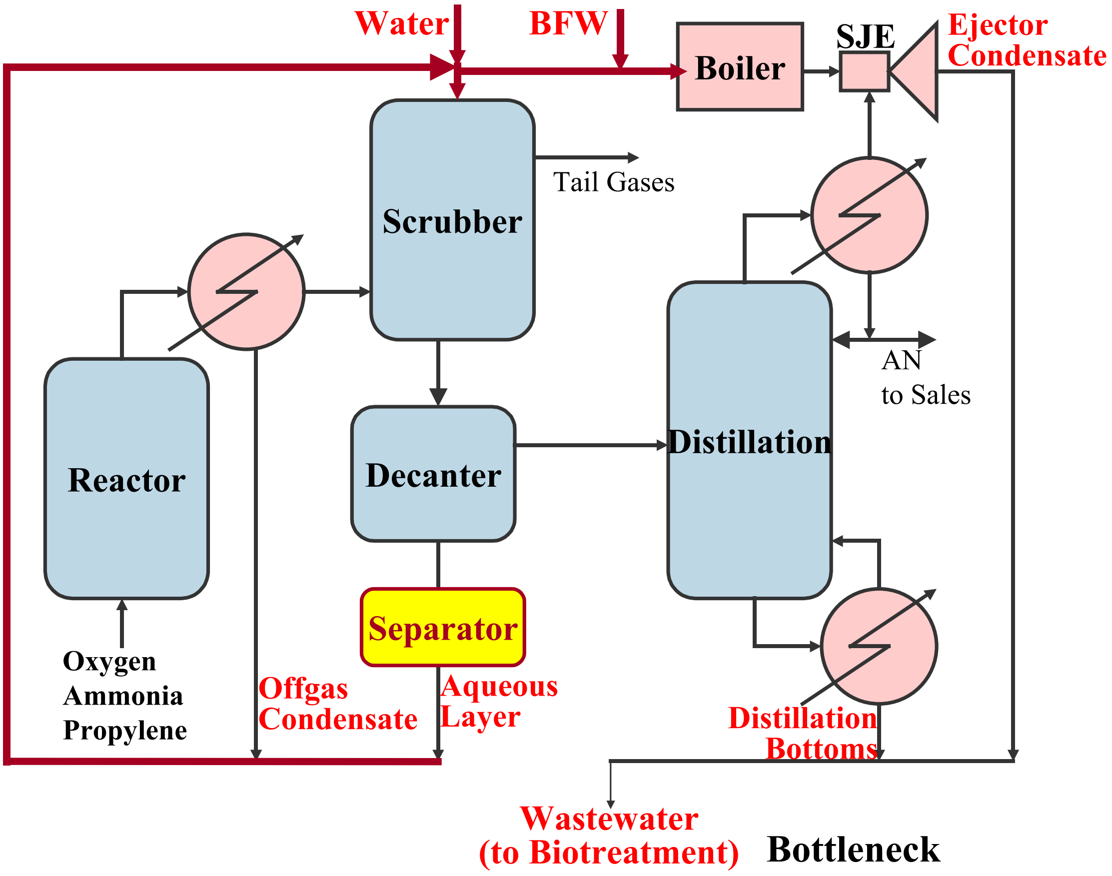

Fig. 1g. Combined Separation and Recycle

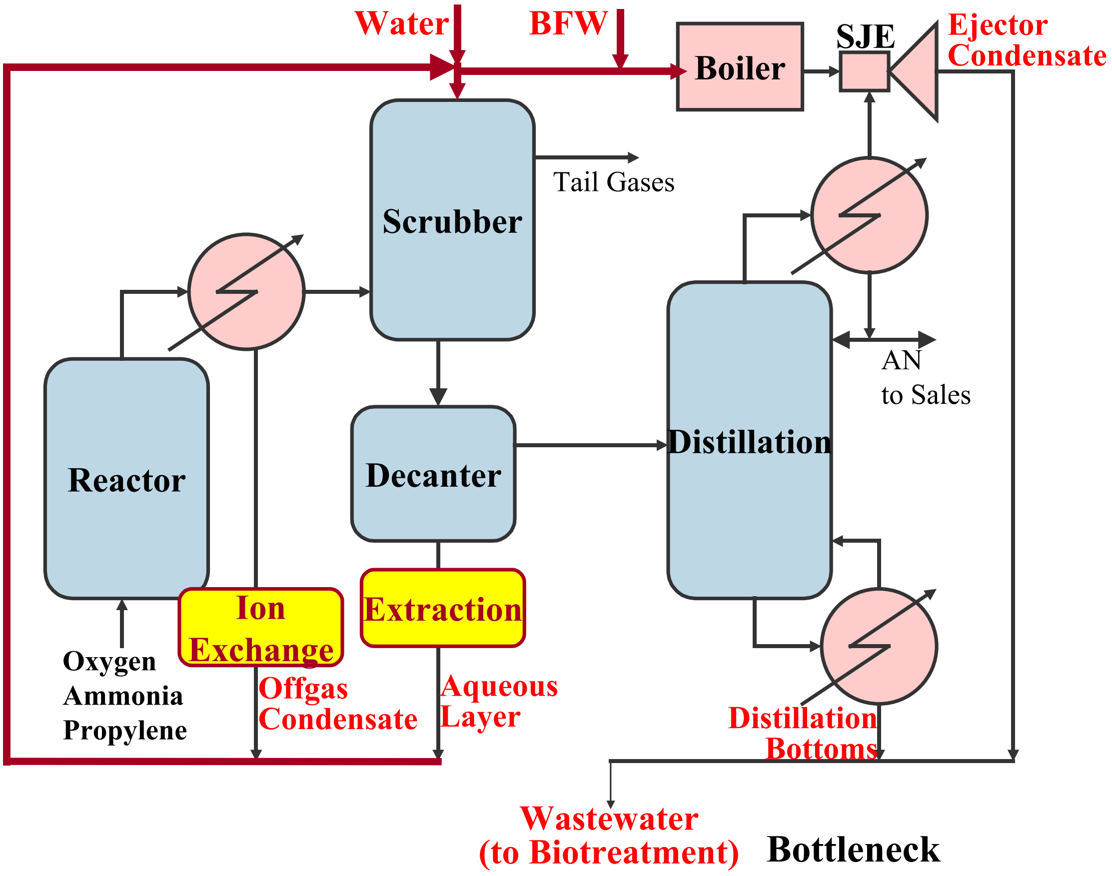

Fig. 1h. Defining Separation Technologies

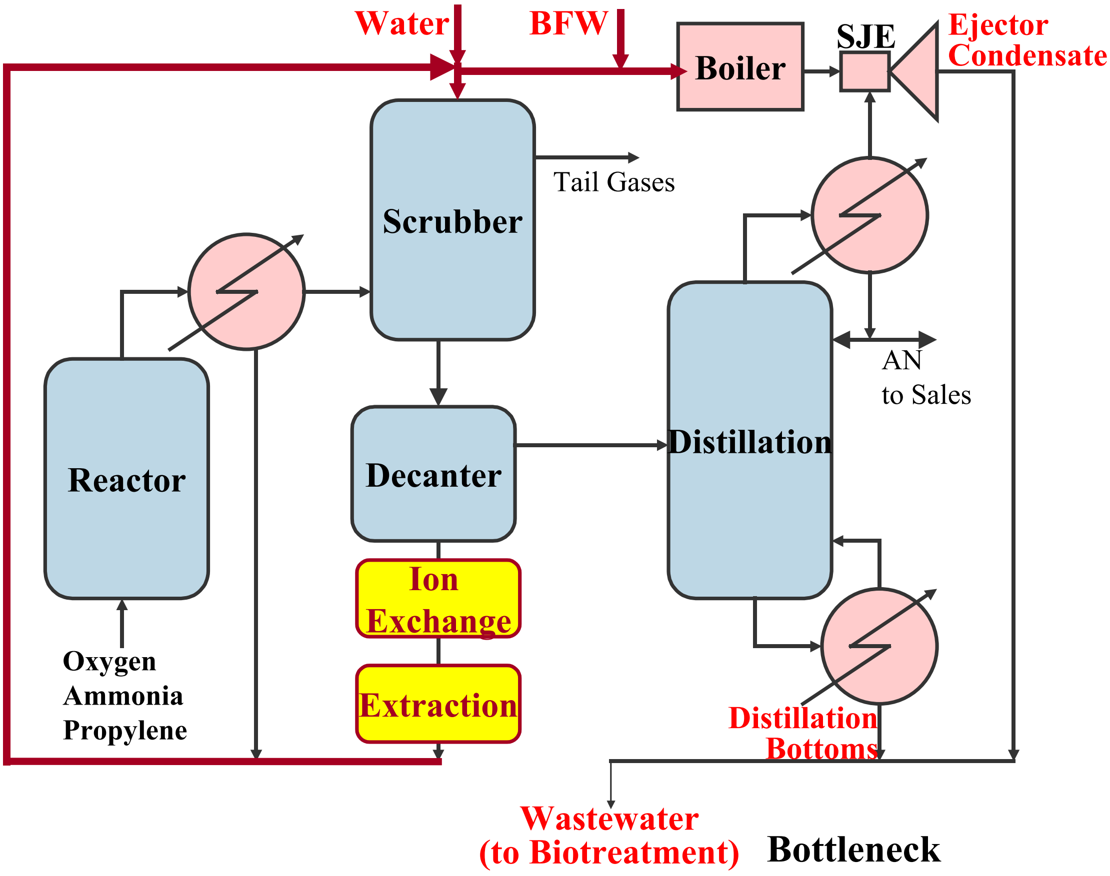

Fig. 1i. Hybrid Separation Technologies for the Decanter Wastewater

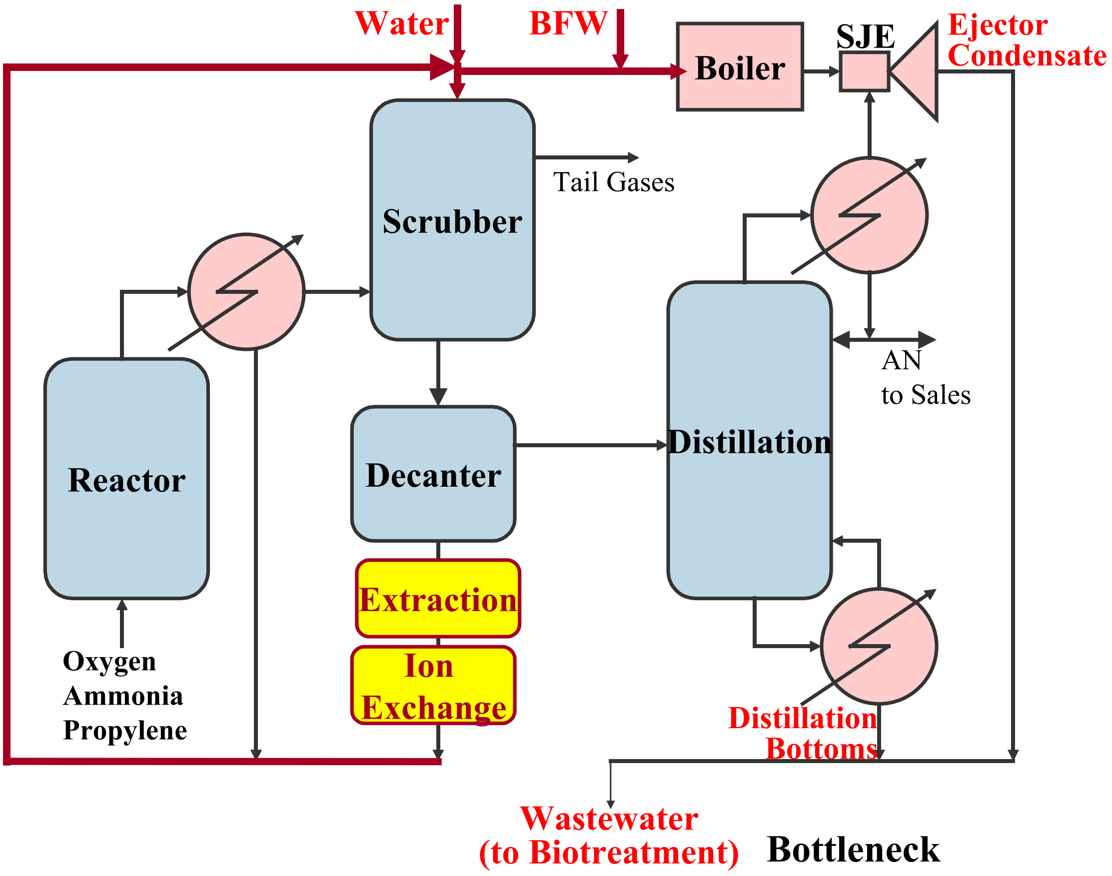

Fig. 1j. Switching the Order of Separation Technologies

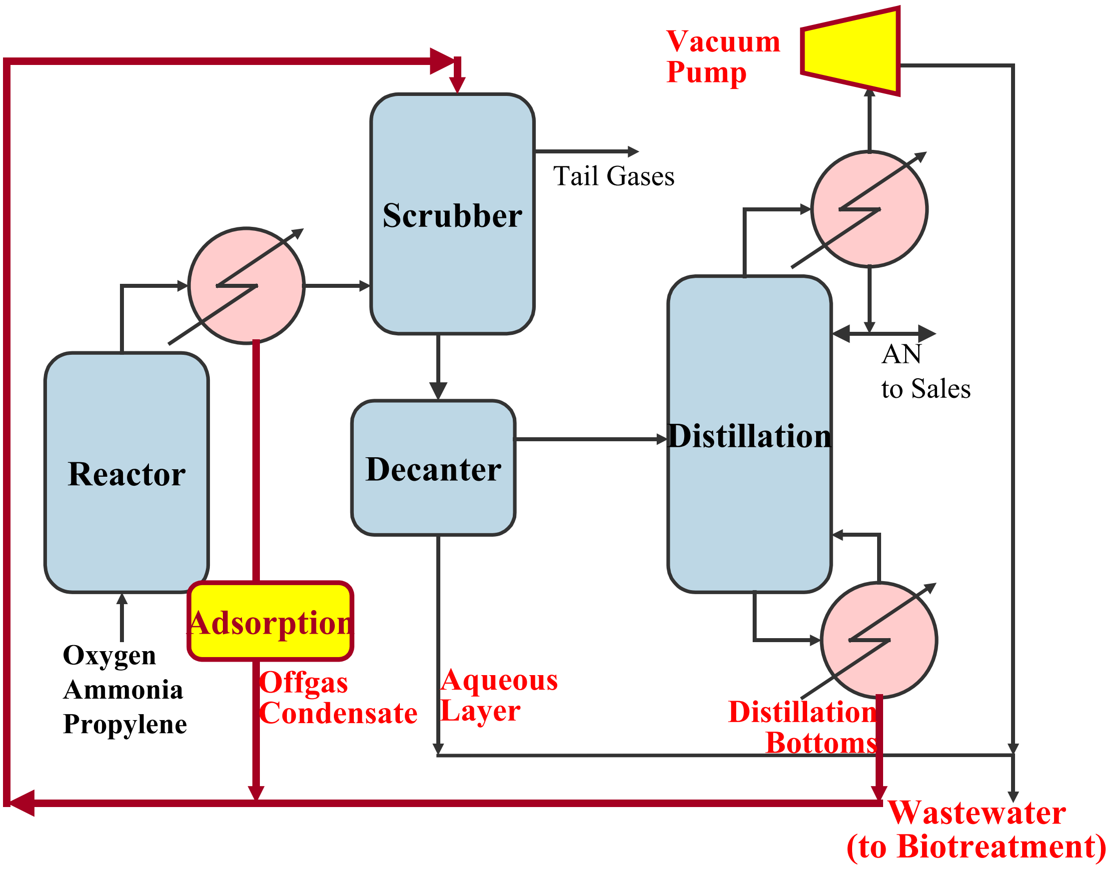

Fig. 1.k. Optimal Solution to AN Case Study

The following observations may be inferred from the foregoing discussion:

- There are typically numerous alternatives that can solve a typical challenging process improvement problem
- The optimum solution may not be intuitively obvious
- Once should not focus on the symptoms of the process problems. Instead, one should identify the root causes of the process deficiencies
- It is necessary to understand and treat the process as an integrated system
- There is a critical need to systematically extract the optimum solution from among the numerous alternatives without enumeration.

## 1.2. TRADITIONAL APPROACHES TO PROCESS DEVELOPMENT AND IMPROVEMENT

Until recently, there were three primary conventional engineering approaches to addressing process development and improvement problems:

- **Brainstorming and Solution through Scenarios**: A select few of the engineers and scientists most familiar with the process work together to suggest and synthesize several conceptual design scenarios (typically three to five). For instance, the foregoing exercise of generating alternative for the AN case study falls under this category. Each generated scenario is then assessed (e.g., through simulation, techno-economic analysis, etc.) to examine its feasibility and to evaluate some performance metrics (e.g., cost, safety, reliability, flexibility, operability, environmental impact, etc.). These metrics are used to rank the generated scenarios and to select a recommended solution. This recommended solution may be inaccurately referred to as the “optimum solution” when in fact it is only optimum out of the few generated alternatives. Indeed, it may be far away for the true optimum solution.

- **Adopting/Evolving Earlier Designs:** In this approach, a related problem that has been solved earlier is identified. The problem may be at the same plant or another plant. Then, its solution is either copied, adopted, or evolved to suit the problem at hand and to aid in the generation of a similar solution.

- **Heuristics:** Over the years, process engineers have discovered that certain design problems may be categorized into groups or regions each having a recommended way of solution. Heuristics is the application of experience-derived knowledge and rules of thumb to a certain class of problems. It is derived from the Greek word "heuriskein" which means "to discover". Heuristics have been used extensively in industrial applications (e.g., Harmsen, 2004).

Over the years, these approaches have provided valuable solutions to industrial problems and are commonly used. Notwithstanding the usefulness of these approaches in providing solution that typically work, they have several serious limitations (El-Halwagi and Sikdar, 2001):

- Cannot enumerate the infinite alternatives: Since these approaches are based on brainstorming few alternatives or evolving an existing design, the generated alternatives are limited.
- Is not guaranteed to come close to optimum solutions: Without the ability to extract the optimum from the infinite alternatives, these approaches may not provide effective solution (except for very simple cases, extreme luck, or near-exhaustive effort). Just because a solution works and is affordable does not mean that it is a good solution. Additionally, when a solution is selected from few alternatives, it should not be called an optimum solution. It is only optimum with respect to the few generated alternatives.
- Time and money intensive: Since each generated alternative should be assessed (at least from a techno-economic perspective), there are significant efforts and expenses involved in generating and analyzing the enumerated solutions.
- Limited range of applicability: Heuristics and rules of thumb are most effective when the problem at hand is closely related to the class of problems and design region for which the rules have been derived. However, they must be used with extreme care. In Even subtle differences from one process to another may render the design rules invalid.
- Does not shed light on global insights and key characteristics of the process: In addition to solving the problem , it is beneficial to understand the underlying phenomena, root causes of the problem, and insightful criteria of the process. Trial and error as well as heuristic rules rarely provide these aspects.
- Severely limits groundbreaking and novel ideas: If the generated solutions are derived from the last design that was implemented or based exclusively on the experience of

similar projects, what will drive the "out-of-the-box" thinking that leads to process innovation.

These limitations can be eliminated if these two approaches are incorporated within a systematic and integrative framework. The good news is that recent advances in process design have led to the development of systematic, fundamental, and generally applicable techniques can be learned and applied to overcome the aforementioned limitations and methodically address process-improvement problems. This is possible through *process integration and its vital elements of process synthesis and analysis.*

### 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 1970's 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 is (Johns, 2001): "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 grass-root design of a new plant). This is shown in Fig. 1.2.

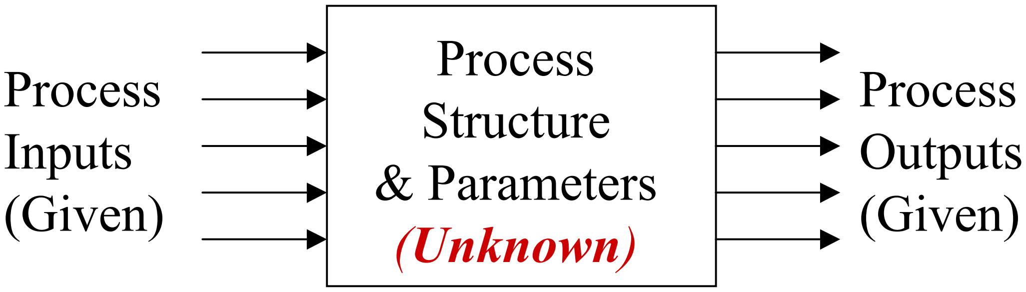

Fig. 1.2. Process Synthesis Problems

Reviews on process synthesis techniques are available in literature (e.g., Westerberg, 2004; Seider et al., 2003; 2001; 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 experiments are 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 (Fig. 1.3).

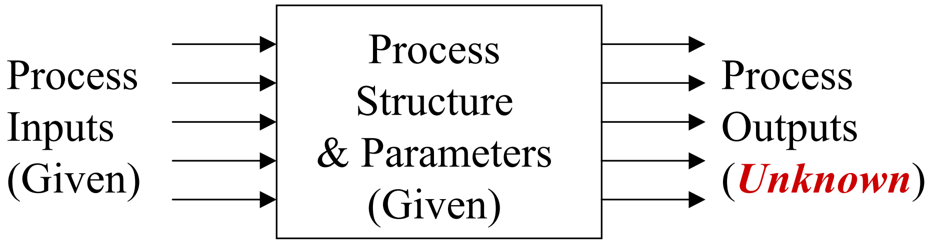

Fig. 1.3. Process Analysis Problem

### 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 Fig. 1.4. The main products are different hydrocarbon cuts. Benzene is further processed in a dehydorgenation 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 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 Fig. 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 in needed to conserve resources and reduce cost.

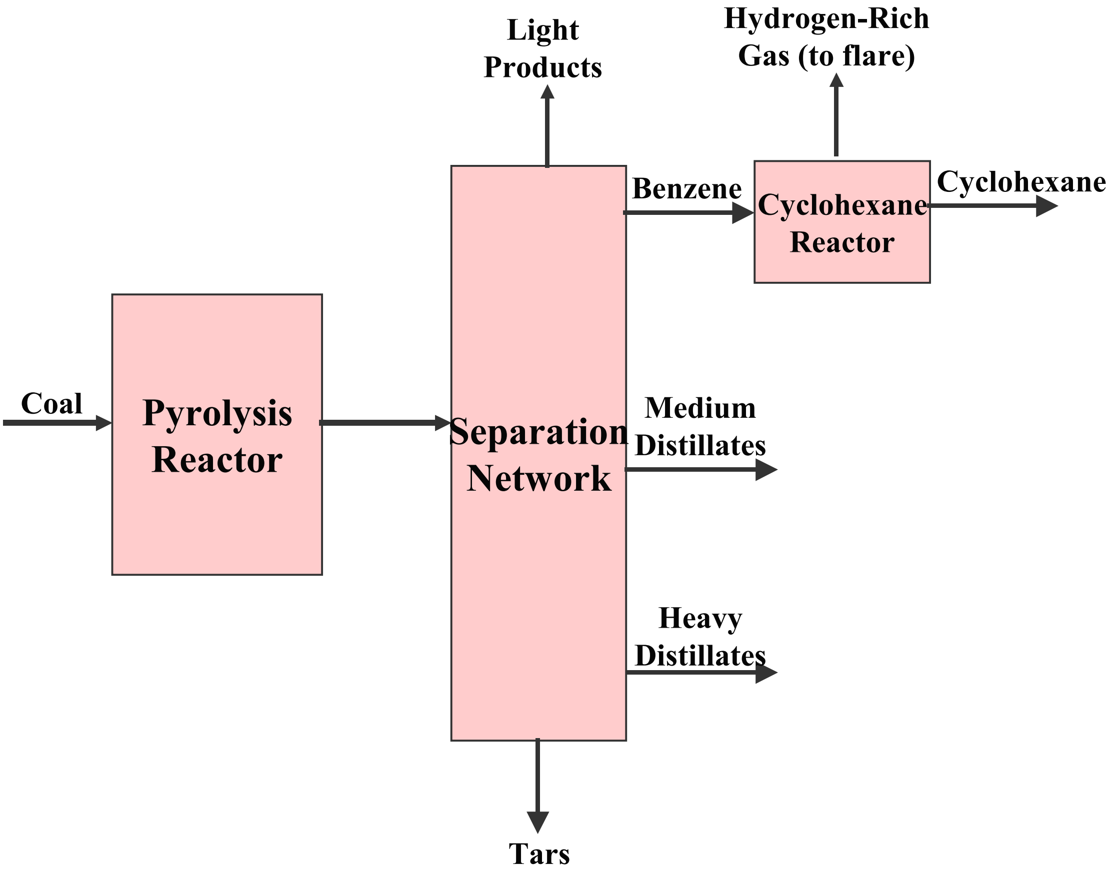

Fig. 1.4. Pyrolysis of Coal

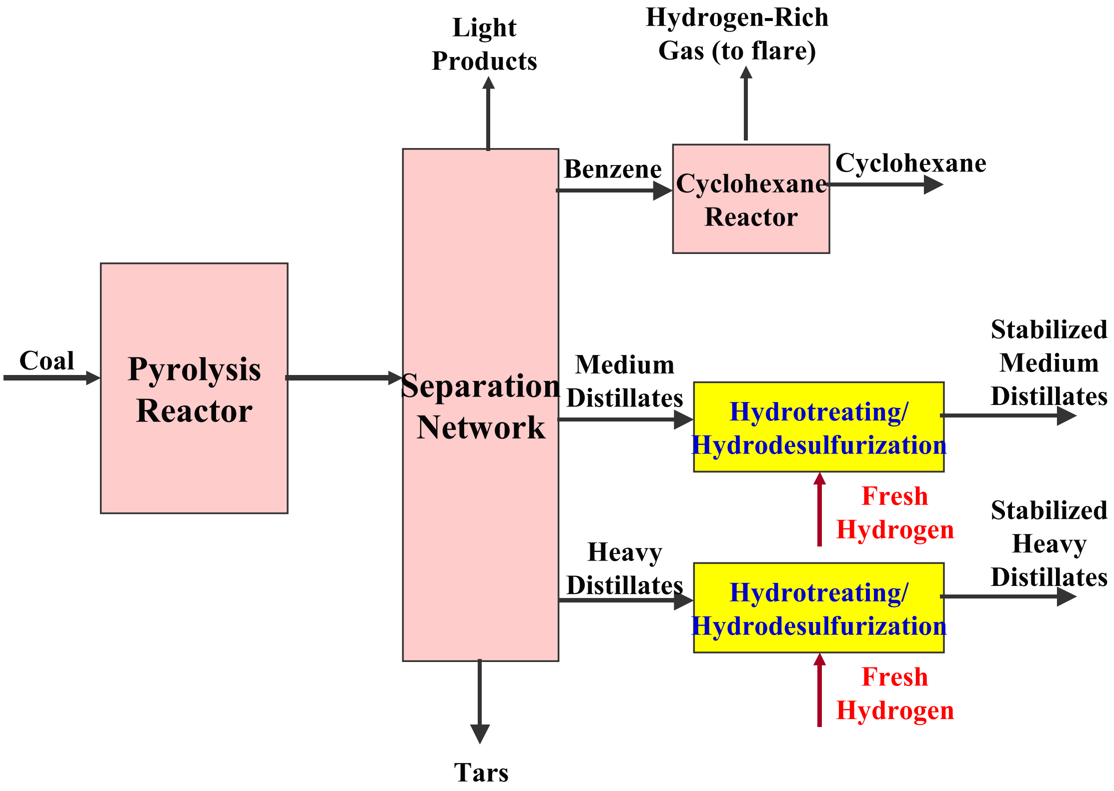

Fig. 1.5. Synthesized Flowsheet for Stabilization of Medium and Heavy Distillates

Reflecting back on the AN case study, the original flowsheet (Fig. 1.1a) suffered from lack of water integration. While fresh water was used in the boiler and the scrubber, waste water 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 Fig. 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. 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.

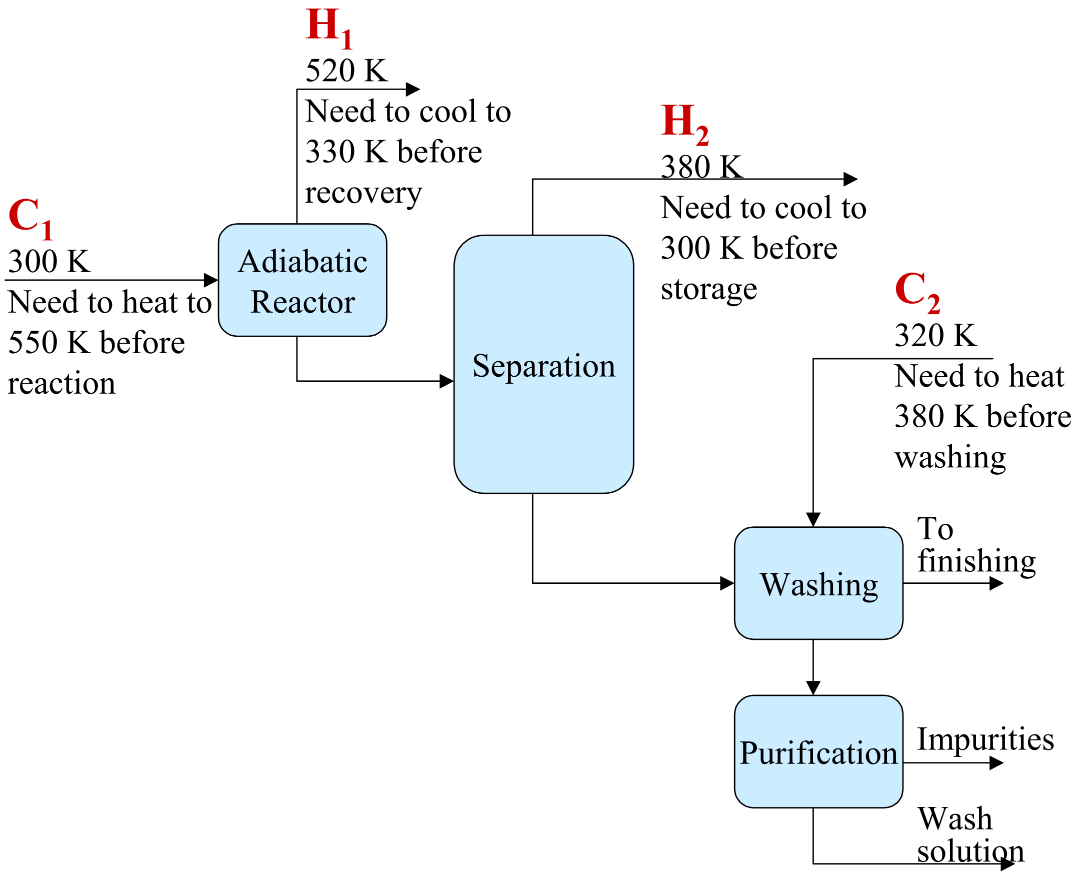

Fig. 1.6. Heating and Cooling Requirements for Pharmaceutical Process (El-Halwagi, 1997)

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 (Fig. 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.

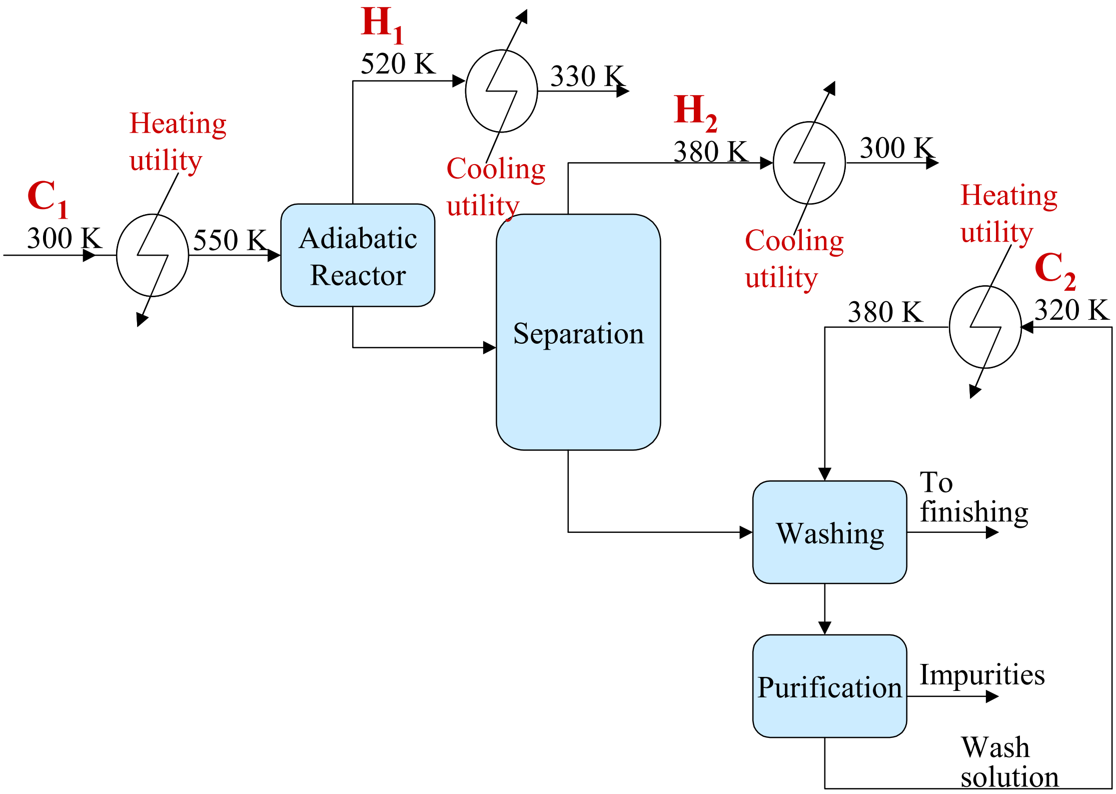

Fig. 1.7. Heating and Cooling Requirements for Pharmaceutical Process (El-Halwagi, 1997)

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.

## 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 will be 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 2,620 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 structural-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 nonlinear 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 intertwined 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 nonlinearity properties of the mathematical formulations mean that obtaining a global solution to these optimization programs can sometimes be an illusive goal. Finally, once the synthesis task is formulated as an MINLP, the engineer's input, preference, judgment, and insights are set aside. Therefore, it is important to incorporate these insights as part of the problem formulation. This can be a tedious task.

## 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 mail 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).

## 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 to illustrate the theories and concepts. It is hoped that this books introduces you to the fascinating world of process integration, concepts, tools, and applications. Welcome aboard!

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