CHAPTER 1

INTRODUCTION

In this first chapter we discuss what process design is all about, some of its history and technical triumphs, and what the future may hold. The essential features of design are summarized, and its vital role in the development of our modern society is discussed.

1.1 OVERVIEW

The function of chemical process design is to take the chemistry that has been discovered by a chemist in small-scale laboratory experiments and end up with a large plant-scale process that efficiently and safely produces large quantities of a useful product. The chemist works with grams of material in test tubes and Parr bombs. The final plant produces millions of kilograms per year of products and requires large equipment (reactors sometimes as large as 100 m^3 and distillation columns 50 m in height and 5 m in diameter). The scale-up factor is often many orders of magnitude.

How the chemist handles the small quantities of chemicals in the laboratory equipment is usually much different from how the engineer deals with the enormous amounts of chemicals in an industrial plant. Basic geometry tells us that the surface-to-volume ratio of a cylinder decreases as the total volume increases. So, as larger and larger reactor vessels are used, the jacket heat-transfer area gets smaller relative to the reaction heat that must be transferred between the jacket and the material in the reactor. Smaller areas require larger differential temperature driving forces for heat transfer, which makes dynamic control more difficult, as we will demonstrate in subsequent chapters. So scale-up is one of the important aspects of process design.

The chemist often conducts batch experiments. Reactants are placed in a test tube and heated to reaction temperature. The changes in composition with time are obtained. The

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effects of the important reaction parameters on these time trajectories are determined: temperature, pressure, initial reactant concentrations, and quantity of catalyst. Kinetic mechanisms are deduced from this batch data, and kinetic relationships and parameters are obtained that fit the experimental data. However, many industrial processes operate continuously, not in batch mode. So the engineer has to use the batch chemical data from the chemist and apply it to continuously operating reactors.

The chemist usually starts with essentially pure reactants and does not worry about separating the mixture of products and reactants that result from the laboratory experiments. These separations are critical to the technical success and economic viability of a large-scale plant. High-purity products must be produced with little variability in product quality. Reactants must be recovered and recycled. By-products must be recovered and disposed of in an economic and pollution-free way.

The separation aspects of a chemical plant often dominate the economics. As many of the case studies presented in subsequent chapters demonstrate, there are important trade-offs between the costs and performance in the reaction section of the process and the costs and performance in the separation section of the process.

The most fundamental process design trade-off is between reactor size and recycle flowrate. The larger the reactor, the smaller the required recycle flowrate. Large reactors increase capital investment in reactor vessels and catalyst. But small recycle flowrates reduce capital investment in separation equipment (distillation columns and heat exchangers) and reduce energy costs in the separation units. So there is a "sweet spot" at which this trade-off gives the "best" flowsheet in terms of economic objectives.

Chemists use nice, pure chemical reactants. The feed streams in many industrial plants frequently are not pure. They can contain chemically inert components that will build up in the unit if not purged out. Undesirable by-products may also be generated that must be removed.

These issues are only a small fraction of the challenges faced by the engineer in developing a process design. The final flowsheet is inevitably a compromise among many competing factors. The process that is built must be economically attractive, it must be safe, and it must be dynamically operable.

This book emphasizes the need to consider both steady-state economics and dynamic controllability through all stages of process development. We call this theology *simultaneous design*. The desirability of combining steady-state and dynamic design has been discussed in process design circles since the pioneering work of Page Buckley at DuPont in the 1950s. Papers and books have been written. Talks have been presented. Symposia have been run. The advantages of coupling design and control have been clearly identified. The simulation tools (software and hardware) are available. Design and control methodology has been developed and documented.

However, it appears that little of this "theology" has been implemented in senior design courses. In almost all chemical engineering departments, process designs are developed with little or no consideration of whether or not the process is controllable. In my opinion, this represents a major flaw in the education of chemical engineers. Old war stories abound of multimillion-dollar plants that have been built but could never be economically and safely operated because of dynamic instabilities.

All the case studies presented in this book combine detailed economics investigations and quantitative dynamic simulation studies. Effective plant-wide control structures are developed that can handle the large disturbances often experienced in industrial processes.

1.2 HISTORY

Chemical process design probably goes back to prehistoric times, when ancient man developed methods for providing food, clothing, and shelter from the raw materials available. The methods and tools were crude by present-day standards, but they were probably considered cutting-edge, high-tech in those days. Making beer and baking bread were (and still are) important chemical processes. Producing soap, tanning leather, and making tools involved crude forms of process design. The Egyptians invented papyrus, the forerunner of paper, way back in 4000 BC.

Chemistry developments built slowly in early civilizations. Copper, bronze, and iron tools and weapons were developed, which facilitated providing food by hunting and tilling the soil. Progress became more rapid through biblical times and the Middle Ages as more and more chemicals were discovered that were useful to mankind. Gunpowder was produced in China around 800 AD. The primary energy source during all these many years was renewable, sustainable, and carbon-neutral wood.

But advances in chemistry accelerated rapidly starting in the eighteenth and nineteenth centuries. Industrial and university chemical research centers were discovering a vast variety of chemicals that had potential value to improve the quality of human life. The production of ammonia for use in agricultural fertilizer produced substantial increases in food production. The Bessemer process for converting iron into steel was developed. Nitroglycerin and TNT were invented. Nobel invented dynamite in 1866. Coal was the primary energy source during this period, and it also was the source of many chemical raw materials. This period was when much coal chemistry was developed.

At the beginning of the twentieth century there was an explosion of activity in chemical process design. Petroleum and natural gas became the principle energy sources as well as the sources of raw materials. The vast variety of hydrocarbons that occur in crude oil or that are produced in refineries in the cracking and reforming processes provided both inexpensive raw materials and energy for the chemical industry.

The intense demands made by two world wars also spurred chemical process design. The development of the atomic bomb in the Manhattan Project relied heavily on a number of complex chemical reaction and separation steps invented by chemical process engineers. The post-World War II expansion of the chemical industry around the world presented enormous challenges and opportunities to process design and control engineers. A drive along the Houston Ship Channel gives some indication of the size of the petroleum and chemical industry. This "mecca" of process design owes it location to cheap gas and oil.

The energy situation has changed drastically in the last several decades. Supply and demand as well as political issues have created rapid increases in gas and oil prices. Most of the new chemical plants are being built in locations that have large gas and oil resources (mostly in the Middle East) or locations with rapidly developing economies (Asia). The need for energy-efficient process design is now more important than ever.

Environmental concerns have also become major drivers in process design. The concern about carbon dioxide emissions has spurred activity in the design of chemical recovery processes for possible sequestration. Reducing the formation of polluting by-products has required significant modifications in many process designs. The new flowsheets feature more extensive recycling to suppress undesirable products or the use of new solvents.

"Times are a-changing" has been an appropriate characterization of process design for many years, and there is no indication that the situation will change. The need for innovative, efficient, economical process design is as strong now as it ever was. So be assured, you are not wasting your time studying and working on process design.

A good process design engineer must have a solid grasp of technical fundamentals, a healthy portion of common sense, a familiarity with practical fluid mechanics (plumbing), the ability to think "out of the box," a strong element of tenacity, and the willingness to work hard.

1.3 BOOKS

The first textbooks dealing with process design began appearing shortly after the formal birth of chemical engineering as a distinct discipline. The 1934 book by Vilbrandt, *Chemical Engineering Plant Design*,[1] appears to be the first textbook dealing with the subject. Topics discussed include mechanical details of equipment and buildings, plant geographic location, and accounting. The 1974 book by Guthrie, *Process Plant Estimating Evaluation and Control*,[2] presented a wealth of material on estimating capital and operating costs in chemical plants. The 1985 book by Peters and Timmerhaus, *Plant Design and Economics for Chemical Engineers*,[3] was the pioneering design text that covered a wide variety of important topics in process design. In 1968, the insightful *Strategy of Process Engineering* by Rudd and Watson[4] developed some of the fundamentals of process flowsheet development. The idea of "conceptual process design" as opposed to "detailed process design" was the result of the pioneering work of Jim Douglas.[5]

A host of textbooks have appeared in recent years that are widely used in senior design courses and represent good reference sources. A partial list is provided at the end of this chapter.[6–13]

However, these books are almost encyclopedic in nature. They attempt to cover all facets of process design, sometimes in excruciating detail. The student finds it difficult to filter out the important "water droplets" from the "ocean" of information and words in these voluminous textbooks. I hope this book is successful in presenting only the essential technical principles that underlie chemical process design.

1.4 TOOLS

There has been tremendous progress in the computational, writing, and graphical tools available for the process design engineer. In the early days of my career (1955), there were only mechanical calculators, slide rules, Leroy lettering sets, and manual typewriters. Computers were not in use by practicing engineers. Engineering calculations were done by hand. Graphical methods were employed where possible. No process simulation software was available.

About this time, analog and digital computers began to appear in industry and in universities. Each company began to develop its own process simulation software. Many large chemical companies (Monsanto, DuPont, Exxon) had proprietary simulators, which could only handle steady-state design.

The Monsanto Company developed FLOWTRAN in the late 1960s. It was made available to universities and other companies in 1973. Over the next several decades a number of process simulators appeared, each with increased capability and improved user-friendliness. Simulators that could handle dynamics and the computers having the required computational speed and memory finally appeared on the scene in the late 1990s.

The current state of process simulation is greatly advanced from where it was fifty years ago. Almost all companies make extensive use of process simulators in both the design and the operation of chemical plants. Steady-state simulation studies are routinely used. A growing number of companies also incorporate dynamic simulations in their design development.

Almost all chemical engineering departments in universities include steady-state process simulation in their design courses. However, it appears that only a tiny handful of departments even mention dynamic plantwide control studies in their design courses. In my opinion, this is a major technical flaw in a design course. To find the "best" design, the dynamic controllability must be investigated.

The advances in other tools have also been enormous. Generating figures in PowerPoint or Visio sure beats struggling with the old Leroy lettering set. Word processing greatly facilitates technical writing. Mathematical tools like MATLAB, MathCad, and Mathematica make technical calculations simple and powerful. Spreadsheets are also widely used.

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