
PRINCIPLES AND CASE STUDIES OF SIMULTANEOUS DESIGN

WILLIAM L. LUYBEN

AIChE[®]

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The book is dedicated to all the past, present and future
Lehigh “kick-ass” engineers.

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PREFACE

Process design involves the development of an effective flowsheet to transform reactants into products in a profitable, safe, environmentally friendly, and controllable plant. Coming up with the best topology of process units is a synthesis problem. It involves science, art, innovation, intuition, inspiration, experience, and common sense. Success also requires a lot of hard work and, at times, a little luck. The designer usually has many criteria to satisfy, many of which are conflicting.

Despite the predictions of many skeptics, chemical process design remains a vital area in chemical engineering. The recognition of the importance of energy and environmental problems, and the interaction between the two, has renewed interest in the design of energy-efficient process plants.

The goal of this book is to present some general design principles in a concise form that should aid the engineer in completing the daunting task of developing an effective flowsheet and control structure. A rich variety of case studies are presented that illustrate in an in-depth and quantitative way the application of these general principles.

Effective development of a chemical process requires the simultaneous consideration of both steady-state economic and dynamic controllability aspects of the process. We call this “simultaneous design.” It is one of the main features of this book.

Detailed case studies are presented of ten complex processes that contain a variety of features commonly occurring in many important industrial plants. In-depth, economic steady-state designs are developed that satisfy an economic objective function such as minimizing total annual cost of both capital and energy. Complete, detailed flowsheets and Aspen Plus files are provided. Conventional proportional-integral (PI) plantwide control structures are developed and tested for their ability to maintain product quality during typically large disturbances. Complete Aspen Dynamics files of the dynamic simulations are provided.

There are many comprehensive design books, but none of them provides a significant number of examples of detailed economic design and accompanying dynamic plantwide control of typically complex industrial processes. Most of the current design books are

“encyclopedic” in nature, in that they cover a very wide spectrum of topics associated with process design. In addition to discussing flowsheet development and equipment design, these textbooks go into a lot of detail in areas that are certainly important but not as technically essential to process design as those presented in this book. The coverage of economics in many of these books includes elegant methods of economic analysis, most of which can hardly be justified by the uncertainties in market predictions. Many chapters in these books are devoted to a host of other somewhat peripheral subjects, such as written and oral skills, ethics, “green” engineering, and product design. The engineer is easily overwhelmed by the sheer size of such a book, and it is difficult to sort out the essentials.

In this book, I intended to cut through this maze of information and present the essential principles of design and control in a brief, readable form that can be easily comprehended by students and engineers in the chemical, petroleum, and biochemical industries. The detailed case studies should provide concrete examples of the application of these design and control principles.

I hope you find this book useful for practical engineering applications and that the subject matter is interesting, important, challenging, and presented in a readable manner. Good luck in your engineering careers. Keep the faith!

WILLIAM L. LUYBEN

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

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 its 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 Watson⁴ 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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CHAPTER 2

PRINCIPLES OF REACTOR DESIGN AND CONTROL

The reaction section of a chemical plant is typically the heart of the process. Here is where the basic chemical transformations of raw materials into products are conducted. The reaction section must be well designed so that the conversion of reactants and the yield of desired products is high, and the dynamic stability of the reactor is guaranteed. Reactors can present major safety and dynamic controllability problems if the reactions are exothermic and irreversible. Many industrial accidents have resulted from poor design and operation of chemical reactors.

In this chapter we discuss basic principles of reactor design and control since the two features are intimately connected. Failure to explore reactor dynamics can lead to catastrophic results.

2.1 BACKGROUND

Reactors occur in many flavors, but we limit our discussion to continuous systems. *Continuous stirred-tank reactors* (CSTR) and tubular reactors are the most common types. The reactors may or may not contain catalysts. The phases in the reactors can be liquid or vapor. The reactors can be adiabatic or involve heat transfer (cooling or heating). Multiple reactors of the same or different types can be operated in series or parallel. The fresh feed streams of reactants can enter the process as gases or liquids.

There are also many types of reactions: endothermic, exothermic, irreversible, reversible, consecutive, simultaneous, homogeneous, heterogeneous, and so on. The type of reaction and the type of reactor exercises a very strong impact on the design of both the reaction section and the separation section of the process.

2.2 PRINCIPLES DERIVED FROM CHEMISTRY

A look at the stoichiometry and the kinetic parameters of the reactions can immediately yield a lot of information about what conditions should be favorable to facilitate the production of desired products. Stoichiometry and the kinetic parameters also determine the general topology of the process in terms of the need for recycles.

2.2.1 Heat of Reaction

Basic kinetics tells us that all specific reaction rates increase with temperature, but chemical equilibrium constants for reversible reactions can either increase or decrease with temperature depending on the heat of reaction.

Endothermic Reactions. Endothermic reactions have positive heats of reaction, so they soak up heat. If the reactor is adiabatic, temperatures will *decrease* from the inlet to the outlet in a tubular reactor. If heat transfer is used in the reactor, heat must be transferred *into* the reactor from a higher-temperature heat source to maintain temperatures.

The chemical equilibrium constant of an endothermic reaction increases as temperature increases. High reactor temperatures increase both specific reaction rates and chemical equilibrium constants. Therefore, conversion is enhanced by running at the highest possible temperature. This means that a small reactor can be used.

So the optimum design of endothermic reactors is relatively easy. You simply operate at the highest possible temperature. Maximum temperature may be limited by a variety of constraints: catalyst degradation, materials of construction, undesirable side reactions that occur at high temperatures, thermal degradation, pressure limitations, and so on.

Many processes with endothermic reaction that operate at high temperatures use multiple adiabatic reactors in series with intermediate furnaces to heat up the process stream to some optimum maximum inlet reactor temperature. The number of reactors and their sizes are important design optimization variables.

Endothermic reactions rarely present control problems. Temperature runaways seldom occur because a temperature increase raises reaction rates, which in turn tend to soak up heat and reduce temperatures. Thus endothermic reactions are self-regulatory.

Exothermic Reactions. Exothermic reactions have negative heats of reaction, so they generate heat. If the reactor is adiabatic, temperatures will *increase* from the inlet to the outlet in a tubular reactor. If heat transfer is used in the reactor, heat must be transferred *out of* the reactor into a lower-temperature heat sink to maintain temperatures.

The chemical equilibrium constant of an exothermic reaction *decreases* as temperature increases. This presents a problem. High reactor temperatures are needed to achieve reasonably large specific reaction rates so that fairly high conversions can be attained. On the other hand, if the temperature is too high, we run into a chemical equilibrium constraint, which means the reaction stops and conversion is limited.

The optimum design of exothermic reversible reactions involves a trade-off between reactor temperature and reactor size. Low temperature can permit high conversion, but a large reactor has to be used. Many processes with this type of reaction are designed with multiple reactors in a series. The first reactors operate at high temperature to get the reactions going. The later reactors operate at lower temperatures so as to avoid the chemical equilibrium constraint.

Reactors with exothermic reactions can present major dynamic control problems. If the exothermic reactions are *reversible*, temperature runaways are usually not an issue because of the self-regulation wrapped up in the chemical equilibrium constraint. If a temperature increase occurs, heat will be generated, which will increase temperature further. However, at some point the forward and the reverse reaction rates will approach each other. The net reaction rate will go to zero, and the temperature will stop climbing.

However, if the exothermic reactions are *irreversible*, there is the potential for temperature runaways. So the system that can present difficult dynamic control problems is one in which the reactions are *irreversible* and *exothermic*. If a temperature increase occurs, heat will be generated, which will increase temperature further and result in a further increase in reaction rate and heat generation. Open-loop unstable reactors can occur and can run away to dangerously high temperature levels. Pressure will build up, safety valves or rupture disks will open, and serious safety and pollution problems may result.

The other necessary ingredient for this instability scenario is a reactor that is operating at low to modest levels of conversion. If the conversion is very high, the concentration of reactant in the reactor will be low. There is very little “fuel” around to cause the reactions to run away. The small amount of reactant will be consumed before dangerous temperatures are reached. This limiting reactant condition is frequently used to provide concentration self-regulation in reaction systems with two reactants and very large activation energies. The high temperature sensitivity can be mitigated by running with only a small concentration of one of the two reactants.

2.2.2 Reversible and Irreversible Reactions

Some aspects of reversible and irreversible reactions have been discussed in the previous section. The impact on reactor design and control was examined. However, the distinction between the two types of reactions also has a strong effect on the topology of the process flowsheet.

Reversible. If the reactions are reversible, it is almost always necessary to design a plant with recycles. The reactor effluent will always contain reactants, which must be recovered and recycled because of the strong economic impact of reactant cost. Therefore the flowsheet with a reversible reaction has one or several recycle streams. The number of recycle streams depends on the number of reactants and the methods used for separating them from the products.

For example, suppose the chemistry is the reversible reaction $A + B \rightleftharpoons C$ and suppose distillation is used to separate the reactor effluent containing all three components. If the volatilities of A and B are larger than C, a single distillation column can be used with a single recycle stream (the distillate) containing A and B. On the other hand, if the volatilities are such that A is the lightest, C is the intermediate, and B is the heaviest, two distillation columns and two recycle streams will be required. Using the direct separation sequence, a recycle stream of A would be taken overhead in the first column and a recycle stream of B would come from the bottom of the second column.

Irreversible. If the reactions are irreversible, high conversions can be attained if reactor temperature and/or reactor size can be made large enough. Reactor temperatures have constraints, as mentioned in the previous section. If the specific reaction rate is still small at this maximum temperature, a very large single reactor would be required to achieve

high conversion. Using multiple reactors in series with decreasing reactant concentrations in successive stages would reduce total volume requirements.

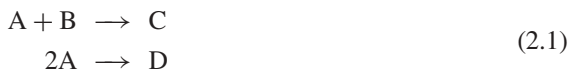
In some cases, the achievable conversions can be high enough to not require any recycle streams. Essentially all of the reactants are consumed. However, in many situations, it turns out to be more economical to use a flowsheet topology with smaller reactors and a separation section with recycle even when the reactions are irreversible.

2.2.3 Multiple Reactions

In most processes, more than just a single reaction occurs. Some reactions are good, making the desired product. Some reactions are bad, making undesired by-products that reduce the yield of the desired product and thereby waste reactant and present expensive waste-disposal problems.

In this section we consider a number of common situations. The desirable and undesirable reactions can be simultaneous or consecutive.

Simultaneous Reactions. Consider the hypothetical reaction system with two simultaneous reactions:



Component C is the desired product. Component D is the bad guy. Looking at this stoichiometry, it is immediately obvious that we need to keep the concentration of A in the reactor low so as to suppress the production of D. The implication of this observation is that we need a large excess of component B to keep the concentration of A small. Therefore the flowsheet topology must include a recycle stream of component B.

For a given reactor temperature, there is a trade-off between the yield of C and the amount of B recycle. If the undesired product D is difficult to get rid of or presents a safety or environmental hazard, we want to make a very small amount of it. Therefore a large B recycle must be used. The capital and energy cost of the separation section and the cost of the reactant raw materials have to be balanced by the costs and risks of handling and disposing of component D.

Of course reactor temperature can also affect conversions and yields. The optimum reactor temperature depends on the activation energies of the two reactions. If the activation energy of the desirable reaction is larger than the activation energy of the undesirable reaction, high reactor temperatures improve yield. If the situation is reversed, low reactor temperatures improve selectivity (more C is made compared to D). However, if reactor temperatures are too low, the specific reaction rate is so small that reactant conversion is low unless very large reactors are used.

The latter situation is very common: low temperatures favor the desired product. So many process designs require trade-offs among the design optimization variables of temperature, reactor size, and recycle. This is a common theme in many of the process case-studies presented in later chapters of this book.

Consecutive Reactions. Consider the hypothetical reaction system with two consecutive reactions:



Component C is the desired product, and component D is the undesired product. It is again obvious that the concentration of component A must be kept small. So all the ideas presented in the previous section also apply in these types of reactions.

Reactor temperature selection depends on the relative values of the two activation energies. The same trade-offs among temperature, size, and recycle apply.

2.3 PRINCIPLES DERIVED FROM PHASE OF REACTION

Reactions occur in either the liquid phase or the gas phase. Liquid-phase reactions are carried out in either CSTRs or tubular reactors. Typical residence times vary from a few minutes to tens of minutes because reactor mass hold-up can be fairly large due to the high liquid density. Most gas-phase reactions are carried out in tubular reactors, since you cannot stir gas. Typical residence times are seconds because of the small vapor density.

Having liquid-phase reactions implies liquid feed streams into the reactor and liquid recycle streams. Having vapor-phase reactions implies gas streams entering and leaving the reactor. The original fresh feeds and the recycle streams to a gas-phase reactor can be either liquid or vapor. If they are liquid, they must be vaporized and preheated to the required reactor inlet temperature in heat exchangers. Attempting to both vaporize and superheat a liquid stream can lead to severe hydraulic problems due to slug flow during the transition from liquid to vapor. These problems can be avoided by using a separate heat exchanger (kettle reboiler) as a vaporizer, which generates saturated vapor, and then a downstream heat exchanger to superheat the gas to the desired reactor inlet temperature.

Fluid mechanics tells us that orders of magnitude less energy is required to pump a liquid than to compress a vapor. So, if a reactor feed stream needs to be a high-pressure gas and if it is originally a liquid, the liquid stream should be pumped up to the required pressure and then vaporized. If the recycle stream is a gas and must be compressed, the pressure drops through the reactor and other units in the gas recycle loop should be kept as small as possible. There is an engineering trade-off between compression costs needed to provide enough pressure drop (velocity) in heat-transfer units for reasonable heat-transfer coefficients and the capital cost of heat exchanger area. Since heat-transfer film coefficients are small in gas systems, heat exchangers tend to be quite large compared to liquid systems in which higher heat-transfer coefficients can be attained by providing more pressure drop, which is inexpensively provided by pumping.

Another aspect of gas-phase reactions is the selection of which reactant to design for high per-pass conversion. Consider the reversible gas-phase reaction $A + B \rightleftharpoons C$, where B is a high-boiling component that is supplied in the liquid phase, while A is a low-boiling gas. There must always be some reactant in the reactor effluent, since the reaction is reversible and complete conversion of both reactants is not possible.

We could design the process for a high conversion of A or a high conversion of B. Which is better? If we feed an excess of A, there will be lots of A coming out of the reactor. This component is a low-boiling component and cannot be condensed inexpensively using cooling water, so a gas recycle stream of A will have to be compressed, which is expensive. Alternatively we could feed an excess of B. This is a high-boiling component that can be condensed and pumped up to the required pressure before vaporizing. Pumping is inexpensive. Vaporization requires significant energy but it may be at a low enough temperature to require relatively inexpensive low-pressure steam. Compression requires high-level energy (electric power or high-pressure steam) that is expensive. So the question of which

is better depends on the relative costs and amounts of energy and capital required in the two alternatives.

Gas-phase systems that require compression are unavoidable in many processes. The work required to compress a gas from a suction pressure P_1 to a discharge pressure P_2 is a minimum if the compression is isothermal. But compressors operate adiabatically. So the design of a gas compressor configuration usually involves a series of compressors and intercoolers. After the first stage of compression, the gas is cooled to as low a temperature as attainable with cooling water in a heat exchanger. Remember that the adiabatic compression of an ideal gas is given by the following equation.

$$W = \frac{\gamma RT_1}{\gamma - 1} \left[\left(\frac{P_2}{P_1} \right)^{\gamma-1/\gamma} - 1 \right] \quad (2.3)$$

The suction temperature T_1 directly affects the work, so the compressor system should be designed for low inlet temperatures. The number of compression stages used is a balance between energy costs and capital investment in compressors and heat exchangers. A useful heuristic in a system with N stages of compression, with an initial feed pressure of P_0 and a final pressure of P_N , is to make the compression ratio in each stage $(P_N/P_0)^{1/N}$.

2.4 DETERMINING KINETIC PARAMETERS

The most difficult part of any process design and the essential simulation is getting reliable reaction kinetic parameters. The commercial simulators provide almost none of this type of data in their libraries, so the designer must go to the laboratory or the literature or the pilot plant or the operating plant to find information.

Using reliable laboratory data in which you have confidence is clearly the most desirable approach. But in many situations, particularly at the conceptual design stage, the process designer must rely on literature data. This can be a real pain, since authors report their results using a variety of units, and the process simulators often require very specific units. The Aspen Plus simulator used in this book requires that overall reaction rates must be given in either “kmoles per second per cubic meters of reactor volume” or “kmoles per second per kilogram of catalyst” in the reactor. Also, if concentrations are given in partial pressures, they must be in terms of Pascals. Translating literature data into these units is not a trivial job but can be speeded by using MathCad or other equation-manipulating software.

2.4.1 Thermodynamic Constraints

The first thing to investigate for any reaction system is the chemical thermodynamic constraints. Using AspenTech software, this is easy to achieve by using the RGIBBS reactor model, which minimizes the free energy of the system to solve for the concentration of reactants and products at chemical equilibrium. Clearly no kinetic reactions can give conversions greater than this.

Place the RGIBBS reactor on the Aspen Plus flowsheet and connect a feed stream of reactants. Specify temperature and pressure, and the model will predict the compositions leaving the reactor. These results are independent of reactor size and would be obtained if