Chemical Process Analysis: Mass and Energy Balances

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Preface

This book is intended for use in a first-level course in chemical engineering. Its basic objectives are: (1) to introduce beginning students to the field of chemical engineering, and (2) to teach the principles of mass and energy balances in the context of designing and operating a chemical process in the most profitable and safest manner.

The book represents a new approach to introduce students to chemical engineering. Its origins go back almost a decade to our dissatisfaction with the first chemical engineering course here at Lehigh. This course covered the topics normally presented in the traditional "stoichiometry" course.

We found, however, that many of our students were not getting a clear picture of what chemical engineering was all about until they took a junior-level "unit operations" course. Thus, some students found out much too late that they really didn't want to be chemical engineers. Some students were also poorly motivated during their sophomore year. Therefore, we searched for some way to move some of this "unit operations" material down into the first sophomore chemical engineering course.

The objective was to provide a course that would permit students to get a good "feel" for chemical engineering at an early stage. This would better motivate those students who liked the material to put in the time and effort it takes to make it successfully through the tough chemical engineering curriculum.

The philosophical basis for this approach was provided by the early book of Thibaut Brian, *Staged Cascades in Chemical Processing* (Englewood Cliffs, NJ: Prentice-Hall, 1972). We found the thrust of this book to be what we were looking for. However, Brian's book was short on quantitative technical material and contained no discussion of solutions to problems by computer techniques.

Accordingly, we began to put together a set of notes that covered much more material. After several revisions, we found that we could effectively cover mass and energy balances applied to three typical and very important staged operations. We could go into enough depth for students to appreciate the challenges and opportunities that a career in chemical engineering has to offer. Quantitative approaches to solving problems, examination of the many alternative process configurations, safety considerations, economics, and engineering compromises were all naturally and effectively covered by examining the staged operations of binary distillation, liquid-liquid extraction, and evaporation.

This unique approach also meant that the number of staged operations topics left to be covered in the unit operations courses was much reduced, permitting more time in these courses for other important material.

We have tested and honed this approach for almost ten years here at Lehigh, revising and fine-tuning our notes almost yearly. Our experience has been very positive. We feel that students leave the course with a good idea of what chemical engineering is and with the quantitative ability to apply mass and energy balances to any new process. The students who stay in the curriculum are better motivated and have a better perspective on how their subsequent courses fit into the chemical engineering knowledge base.

We recognize that this book is a break with tradition. We feel it is an exciting and effective new approach and hope you will give it a try.

The contributions of many people to the development of the book are gratefully acknowledged. Certainly, first on the list should be the many bright-eyed and bushy-tailed sophomores who have suffered through many revisions. Their incisive and sometimes painfully candid comments were invaluable. We thank Mike Luyben for proofreading the final version of the manuscript. Our colleagues Hugo Caram, Cesar Silebi, and Bryce Andersen also deserve thanks for team-teaching the course with us on several occasions. Jane Lenner was a model of thoroughness and patience in typing the many revisions of the manuscripts. Kathy Turoski helped in the final typing.

Finally, we would like to thank our families for their support and encouragement over some fifty years of collective teaching careers. All the crack-of-dawn and late-evening writing periods would have been impossible without a lot of understanding and love. We officially apologize for all of the times we got home late for dinner!

This book is dedicated to the memories of two outstanding engineers and teachers: Alan S. Foust and Jack A. Gerster.

William L. Luyben
Leonard A. Wenzel

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The Chemical Engineering Profession 1

1.1 WELCOME AND OVERVIEW

Welcome to chemical engineering! If you are the typical reader of this book, you are a sophomore taking your first course in chemical engineering. You may have some doubts and many questions about what you are getting yourself into by tackling this curriculum. You need to learn more about the profession quickly in order to decide whether or not you should "tough it out" in a course of study that is correctly reputed to be difficult and demanding.

What are you getting yourself into? Well, the purpose of this book and the course that you are taking is to provide answers to some of your questions. The book has two basic objectives:

1. *To introduce beginning students to the field of chemical engineering.* Many students know very little about what chemical engineers do, where they work, how much money they make, and the like. Chapters 1 through 3 attempt to describe some typical chemical processes and typical chemical engineering activities. We strongly recommend that this material be supplemented by plant trips (to see, feel, and smell a chemical plant or oil refinery) and by talks from practicing chemical engineers (alumni of your school are particularly effective since they demonstrate that it is possible to get through the curriculum). Both are invaluable to inexperienced students in gaining some concept of the size and complexity of a modern chemical plant and in providing a perspective of the wide variety of career potentials available to chemical engineers.

2. *To teach the principles of mass and energy balances in the context of designing and operating a chemical process in the most profitable and safest manner.* These basic principles are presented along with a large number of examples and problems that illustrate their use both for processes that include chemical reactions and for those that do not. We have chosen to illustrate the application of the principles by analyzing in a fair amount of detail three relatively simple but extremely important countercurrent staged operations: distillation, evaporation, and extraction. These staged processes are very widely used in industry and are reasonably easy for a beginning student to understand. Therefore, sufficiently detailed knowledge can be gained in a beginning course to permit introduction to (1) the design and operating trade-offs that are so typical in chemical engineering, (2) a consideration of safety and economics, and (3) comparisons of alternative process configurations.

We hope this book will give you a "feel" for the field of chemical engineering early in your college career. The material includes both the traditional graphical solution techniques (McCabe-Thiele and Ponchon diagrams) as well as the more modern computer solutions. Mass and energy balances for multistaged processes are ideally suited for digital computer solutions; the computer permits you to solve difficult problems without having to make too many simplifying assumptions, and it allows you to explore a large number of process cases (e.g., different quantities and compositions of feed streams, different desired products, and alternative process configurations).

Please heed a well-intended word of warning about the use of computers in engineering: they are very powerful tools, but they are only as smart as the engineers who use them. Students sometimes get so wrapped up in *computing* that they stop *thinking*! You have to understand the basic fundamentals and the engineering aspects of a problem before you can effectively use a computer. That is why the computer solutions are given after the basic concepts have been learned. The traditional graphical methods are presented first because they show a picture of what is going on as process parameters are changed. Once this insight has been gained, you are ready to go to the computer for more rigorous and extensive calculations.

The material in the book is basically very simple. By the time you are juniors and seniors, you will look back on this material (fondly, we hope!) as being straightforward common sense. However, you will not find it easy as you go through it for the first time. The typical beginning student finds the first course in chemical engineering difficult for a couple of reasons:

1. You have to learn a new language, including many new terms that you must understand and remember. For example, what is a "tube-in-shell heat exchanger"? What do terms like "relative volatility" and "reflux ratio" mean? All this chemical engineering jargon takes

time and effort to assimilate. In addition, you must learn English engineering units. You are familiar with metric units and the SI system from your chemistry and physics courses. But many people in industry still use English units. So you must learn the language of "pounds," "feet," degrees "Fahrenheit" and "Rankine," "psig," "psia," "gpm," etc. The newer "SI" units (e.g., pressures in "pascals" instead of "psig" and "atmospheres") must also be applied in engineering situations. We will talk more about this later.

2. You will find that most chemical engineering courses are quite different from the science courses you have taken. The objective is not to memorize formulas (most chemical engineering tests are "open book"); rather, the emphasis is on learning to think and to apply basic principles to new situations. You have to learn to derive your own formulas for the specific situation you are dealing with. You simply go back to fundamental mass balances and energy balances. Indeed, the only equation you will need to memorize for this course is

$$\text{IN} = \text{OUT}$$

Sound simple? Well, it is, but it takes a little practice and sweat to get the hang of it. Once you get the idea, though, you will wonder why it took you so long to learn.

1.2 HISTORY

The chemical industry developed in Europe, especially in Germany, toward the end of the nineteenth century. The United States imported what few chemicals were used here, especially dyes and simple drugs. There was a small U.S. chemical industry making explosives and some of the more basic inorganic chemicals, refining metals, tanning leather, and assisting in papermaking. The mounting tensions as World War I approached, and the war itself, cut off the U.S. from easy access to Germany. Suddenly, a chemical industry had to be built here.

In Germany, industrial chemical operations were built and managed by mechanical engineers working with industrial chemists. That pattern has been retained almost to the present. In the U.S., however, few chemists existed, and they did not relish a shift from their laboratories. Nor did mechanical engineers in the U.S. have the classical background in chemistry afforded by the rigorous secondary school system of Europe. Instead, the basic principles were being evolved by faculty in what soon became chemical engineering departments at MIT and Michigan. Such men as A. D. Little, W. K. Lewis, and A. H. White developed the idea that chemical processes could be broken up into (1) unit operations such as heat transfer, distillation, evaporation, and filtration, and (2) unit processes such as oxidation, sulfonation, and nitration. These units could then be studied as separate entities. Because there was a strong need at that time for professionals who were hybrids combining the skills of the chemist and the mechanical engineer, the chemical engineering discipline began to grow.

Through the years, chemical engineers have played a large and vital role in developing the U.S. chemical and petroleum industries. They have served as designers, construction consultants, and operators of chemical plants. They have also been important participants in research and development. The need to learn more about the processing operations themselves and the fundamental mechanisms involved was recognized and pursued. Finally, chemical engineers have assumed a role in the chemical business field in forecasting needs, consulting on product and equipment use, and marketing.

The discipline of chemical engineering has spread throughout the world. Curricula in chemical engineering, closely modeled after those in the U.S., are to be found on all the continents.

1.3 CURRICULUM

As chemical engineering knowledge developed, it was inserted into university courses and curricula. Before World War I, chemical engineering programs were distinguishable from chemistry programs in that they contained courses in engineering drawing, engineering thermodynamics, mechanics, and hydraulics taken from engineering departments. Shortly after World War I the first text in unit operations was published (W. H. Walker, W. K. Lewis, and W. H. McAdams, *Principles of Chemical Engineering*, New York: McGraw-Hill, 1923). Courses in this area became the core of chemical engineering teaching.

By the mid-1930s, chemical engineering programs included courses in (1) stoichiometry (using material and energy conservation ideas to analyze chemical process steps), (2) chemical processes or "unit operations," (3) chemical engineering laboratories (in which equipment was operated and tested), and (4) chemical plant design (in which cost factors were combined with technical elements to arrive at preliminary plant designs). The student was still asked to take the core chemistry courses, including general, analytical, organic, and physical chemistry. However, in addition, he or she took courses in mechanical drawing, engineering mechanics, electric circuits, metallurgy, and thermodynamics with other engineers.

Since World War II chemical engineering has developed rapidly. As new disciplines have proven useful, they have been added to the curriculum. Chemical engineering thermodynamics became generally formulated and taught by about 1945. By 1950, courses in applied chemical kinetics and chemical reactor design appeared. Process control appeared as an undergraduate course in about 1955, and digital computer use began to develop about 1960.

The idea that the various unit operations depended on common mechanisms of heat, mass, and momentum transfer developed about 1960. Consequently, courses in transport phenomena assumed an important position as an underlying, unifying basis for chemical engineering education. New general disciplines that have emerged in the last two decades include environmental and safety engineering, biotechnology, and electronics manufacturing processing. There has been an enormous amount of development in all fields, much of it arising out of more powerful computing and applied mathematics capabilities.

The new subjects forced some cuts in the non-chemical engineering part of the curriculum. Peripheral engineering courses were reduced, but the chemistry content of most curricula has remained strong. The reduction in the former areas was possible because of improved student preparation in high school science and mathematics. In fact, the number of courses in humanities and social sciences has actually increased, since it has been recognized that social, political, and human factors are vitally important in designing and operating a chemical process.

We suggest that you look at your college catalog and review the chemical engineering curriculum at your school. It will give you some perspective of where you are going and what courses you will be taking.

1.4 TYPICAL ACTIVITIES

The classical role of the chemical engineer is to take the discoveries made by the chemist in the laboratory and develop them into money-making, commercial-scale chemical processes. The chemist works in test tubes and Parr bombs with very small quantities of reactants and products (e.g., 100 ml), usually running "batch," constant-temperature experiments. Reactants are placed in a small container in a constant-temperature bath. A catalyst is added and the reactions proceed with time. Samples are taken at appropriate intervals to follow the consumption of the reactants and the production of products as time progresses.

By contrast, the chemical engineer typically works with much larger quantities of material and with very large (and expensive) equipment. Reactors can hold 1,000 gallons to 10,000 gallons or more. Distillation columns can be over 100 feet high and 10 to 30 feet in diameter. The capital investment for one process unit in a chemical plant may exceed $100 million!

Many commercial processes run in a "continuous" mode, as opposed to the "batch" mode that the chemist almost always employs. Feed streams and product streams are continuously fed and withdrawn from the process. The usual goal is to obtain "steady-state" operation in which all parameters in the continuous plant (temperatures, liquid levels, pressures, flow rates, compositions, etc.) are constant with time.

The chemical engineer is often involved in "scaling up" a chemist-developed small-scale reactor and separation system to a very large commercial plant. The chemical engineer must work closely with the chemist in order to understand thoroughly the chemistry involved in the process and to make sure that the chemist gets the reaction kinetic data and the physical property data needed to design, operate, and optimize the process. This is why the chemical engineering curriculum contains so many chemistry courses.

The chemical engineer must also work closely with mechanical, electrical, civil, and metallurgical engineers in order to design and operate the physical equipment in a plant—the reactors, tanks, distillation columns, heat exchangers, pumps, compressors, control and instrumentation devices, and so on. One big item that is always on such an equipment list is piping. One of the most impressive features of a typical chemical plant is the tremendous number of pipes running all over the site, literally hundreds of miles in many plants. These pipes transfer process materials (gases and liquids) into and out of the plant. They also carry utilities (steam, cooling water, air, nitrogen, and refrigerant) to the process units.

To commercialize the laboratory chemistry, the chemical engineer is involved in development, design, construction, operation, sales, and research. The terminology used to label these functions is by no means uniform from company to company, but a rose by any other name is still a rose. Let us describe each of these functions briefly. It should be emphasized that the jobs we shall discuss are "typical" and "classical," but are by no means the only things that chemical engineers do. The chemical engineer has a broad background in mathematics, chemistry, and physics. Therefore, he or she can, and does, fill a rich variety of jobs in industry, government, and academia.

1.4.1 Development

Development is the intermediate step required in passing from a laboratory-size process to a commercial-size process. The "pilot-plant" process involved in development might involve reactors that are five gallons in capacity and distillation columns that are three inches in diameter. Development is usually part of the commercialization of a chemical process because the scale-up problem is a very difficult one. Jumping directly from test tubes to 10,000-gallon reactors can be a tricky and sometimes dangerous endeavor. Some of the subtle problems involved which are not at all obvious to the uninitiated include mixing imperfections, increasing radial temperature gradients, and decreasing ratios of heat transfer areas to heat generation rates.

The chemical engineer works with the chemist and a team of other engineers to design, construct, and operate the pilot plant. The design aspect involves specifying equipment sizes, configuration, and materials of construction. Usually pilot plants are designed to be quite flexible, so that a wide variety of conditions and configurations can be evaluated.

Once the pilot plant is operational, performance and optimization data can be obtained in order to evaluate the process from an economic point of view. The profitability is assessed at each stage of the development of the process. If it appears that not enough money will be made to justify the capital investment, the project will be stopped.

The pilot plant offers the opportunity to evaluate materials of construction, measurement techniques, and process control strategies. The experimental findings in the pilot plant can be used to improve the design of the full-scale plant.

.4.2 Design

Based on the experience and data obtained in the laboratory and the pilot plant, a team of engineers is assembled to design the commercial plant. The chemical engineer's job is to specify all process flow rates and conditions, equipment types and sizes, materials of construction, process configurations, control systems, safety systems, environmental protection systems, and other relevant specifications. It is an enormous responsibility.

The design stage is really where the big bucks are spent. One typical chemical process might require a capital investment of $50 to $100 million. That's a lot of bread! And the chemical engineer is the one who has to make many of the decisions. When you find yourself in that position, you will be glad that you studied as hard as you did (we hope) so that you can bring the best possible tools and minds to bear on the problems.

The product of the design stage is a lot of paper:

1. *Flow Sheets* are diagrams showing all the equipment schematically, with all streams labeled and their conditions specified (flow rate, temperature, pressure, composition, viscosity, density, etc.).
2. *P and I (Piping and Instrumentation) Drawings* are drawings showing all pieces of equipment (including sizes, nozzle locations, and materials), all piping (including sizes, materials, and valves), all instrumentation (including locations and types of sensors, control valves, and controllers), and all safety systems (including safety valve and rupture disk locations and sizes, flare lines, and safe operating conditions).
3. *Equipment Specification Sheets* are sheets of detailed information on all the equipment: precise dimensions, performance criteria, materials of construction, corrosion allowances, operating temperatures

and pressures, maximum and minimum flow rates, and the like. These "spec sheets" are sent to the equipment manufacturers for price bids and then for building the equipment.

Small-scale physical models of the plant are often built to help the engineers visualize and design the plant layout of equipment and piping. If you enjoy model railroading, you'll like to work with miniature plant models. Indeed, the design stage is where a lot of creative and innovative engineering can be translated into a real plant. The decisions made at this stage are long lived and very expensive to modify later in the field after the plant is built.

1.4.3 Construction

After the equipment manufacturers (vendors) have built the individual pieces of equipment, the pieces are shipped to the plant site (sometimes a challenging job of logistics, particularly for large vessels like distillation columns). The construction phase is the assembling of all the components into a complete plant. It starts with digging holes in the ground and pouring concrete for foundations for large equipment and buildings (e.g., the control room, process analytical laboratory, and maintenance shops). In some soils, pilings must be driven into the ground to support the structures. The technical aspects of these activities are usually handled by civil engineers.

After these initial activities, the major pieces of equipment and the steel superstructure are erected. Heat exchangers, pumps, compressors, piping, instrument sensors, and automatic control valves are installed. Control system wiring and tubing are run between the control room and the plant. Electrical wiring, switches, and transformers are installed for motors to drive pumps and compressors. As the process equipment is being installed, it is the chemical engineer's job to check that it is all hooked together properly and that each piece works correctly.

This is usually a very exciting and rewarding time for most engineers. You are seeing your ideas being translated from paper into reality. Steel and concrete replace sketches and diagrams. Construction is the culmination of years of work by many people. You are finally on the launch pad, and the plant is going to fly or fizzle! The moment of truth is at hand.

Once the check-out phase is complete, "startup" begins. Startup is the initial commissioning of the plant. It is a time of great excitement and round-the-clock activity. It is one of the best learning grounds for the chemical engineer. Now you find out how good your ideas and calculations really are. The engineers who have worked on the pilot plant and on the design are usually part of the startup team.

The startup period can require a few days or a few months, depending on the newness of the technology, the complexity of the process, and the quality of the engineering that has gone into the design. Problems are fre-