Predicting *the* Performance *of* Multistage Separation Processes

Second Edition

Fouad M. Khoury

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Fouad M. Khoury, Ph.D., P.E., is a specialist in multistage separation processes, their modeling and optimization. He is a registered professional engineer in Texas and a member of the American Institute of Chemical Engineers. He received his Ph.D. degree in chemical engineering from Rice University and is the author of numerous articles on multistage separation processes, thermodynamics, and transport phenomena.

Dedication

To my wife Yola
for her encouragement and inspiration,
and countless other contributions,

and to our children, Sami and Nadia,
for their understanding and support.

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Preface

Multistage separation processes are the heart of the petroleum, petrochemical, and chemical industries. These industries yield important products as common as gasoline and plastics and as specialized as medical-grade pharmaceuticals.

This book is aimed at performance prediction of multistage separation processes that is essential for their efficient design and operation. It is distinguished by its emphasis on computer modeling, expert interpretation of models, and discussion of modern simulation techniques. It is also unique in that it relates fundamental concepts to intuitive understanding of processes. A generous number of examples are provided in a wide variety of applications to demonstrate the performance of processes under varying conditions and the relationships among the different operating variables. The book is of value as a reference for practicing engineers in the process industry and for advanced level students of engineering process design.

Improved accuracy in predicting thermodynamic and physical properties has occurred simultaneously with major advances in the development of computational techniques for solving complex multistage separation equations. The result has been the emergence of a variety of simulation programs for accurate and efficient prediction of multistage separation processes. This has provided engineers with valuable tools that can help them make more reliable qualitative as well as quantitative decisions in plant design and operation. Frequently, however, effective use of such programs has been hampered by lack of understanding of fundamentals and limitations of prediction techniques. Improper use of simulators can be costly in time and money, which tends to defeat the purpose of computer-aided engineering. These problems are addressed here, and a strategy is pursued that decouples the discussion of conceptual analysis of the material and the computational techniques.

Although rigorous mathematical methods are presented with a good degree of detail, special attention is given throughout the book to keep practical interpretation of the models in focus, emphasizing intuitive understanding. Graphical techniques and shortcut methods are applied wherever possible to gain a handle on evaluating performance trends, limitations, and bottlenecks. Also included are industrial practice heuristics about what ranges of operating variables will work. The student of this book should come away with an enhanced intuitive grasp of the material as well as a basic understanding of the calculational techniques.

The book may be used for a methodical study of the subject or as a reference for solving day-to-day problems. It follows a logical flow of ideas within each chapter and from one chapter to the next, yet each chapter is quite self-contained for quick reference. The discussion starts with fundamental principles, prediction of thermodynamic properties, the equilibrium stage, and moves on to the different types of multistage and complex multistage and multicolumn processes and batch distillation. Although computer simulation is a central theme of this book, no previous experience in the use of simulation software is required.

Earlier chapters use simplified and binary models to analyze in a very informative way some fundamentals such as the effect of reflux ratio and feed tray location, and to delineate the differences between absorption and distillation. Following chapters

concentrate on specific areas such as complex distillation, with detailed analyses of various features such as pumparounds and side-strippers and when they should be used. Also discussed are azeotropic, extractive, and three-phase distillation operations, liquid–liquid extraction, and reactive distillation. The applications are clearly explained with many practical examples.

Shortcut computational methods, including modular techniques for on-line, real-time applications, are discussed, followed by a discourse on the major rigorous algorithms in use for solving multicomponent separations.

An understanding of column hydraulics in both trayed and packed columns is essential for a complete performance analysis and design of such devices. The reader will find instructional coverage of these topics, as well as of tray efficiency, in subsequent chapters.

Finally, in a departure from steady-state processes that characterize the rest of the book, the subject of batch distillation is discussed. This process, important for separating pharmaceuticals and specialty chemicals, is presented, including shortcut and rigorous computational methods, along with various optimization techniques.

Fouad M. Khoury, Ph.D., P.E.

Preface to the Second Edition

The favorable reception of the first edition in the industry and academic fields has resulted in the publication of this second, enhanced edition of *Predicting the Performance of Multistage Separation Processes*.

The second edition includes several improvements and updates, and, most important, the addition of about 100 application problems and solutions. These exercises expound on the material throughout the book, and can serve both as teaching material and an applications-oriented extension of the book.

The problems cover three major aspects of the learning process: theory and derivation of application equations, engineering and problem-solving cases, and numerical and graphical exercises. The numerical problems require an algorithm definition and computations which may be done manually. For computer-oriented courses, these problems provide excellent material for program writing exercises.

Fouad M. Khoury, Ph.D., P.E.
Houston, Texas
September 1999

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CHAPTER 1

Thermodynamics and Phase Equilibria

The separation processes discussed in this book involve interactions between vapor and liquid phases, or between two liquid phases, or between a vapor phase and two liquid phases. The thermodynamic principles that govern these interactions are introduced in this chapter. Because this chapter is not intended as a full treatise on thermodynamics, only those aspects of the subject that have a direct bearing on phase separation processes are covered. To this end, theory is developed from basic principles and carried through to the formulation of practical methods for correlating relevant thermodynamic properties, such as fugacity and enthalpy. These properties are essential for carrying out heat and material balance calculations in the separation processes described in this book.

When theoretical principles are applied to solve practical problems, various conditions of complexity are encountered. The general approach is to apply the theory to "ideal" systems and then to account for nonidealities by developing models such as equations of state and activity coefficient equations. Models are judged on their consistency with thermodynamic principles and their accuracy in representing actual data. One model may be appropriate for a given system but totally inadequate for another. Hence, the importance of properly selecting a thermodynamic model when attempting to deal with a given separation problem cannot be overemphasized.

1.1 THERMODYNAMIC FUNDAMENTALS

Thermodynamics is a science that relates properties of substances, such as their internal energy, to measurable quantities, such as their temperature, pressure, density, and composition. Thermodynamics also deals with the transformation of energy from one form to another, such as the transformation of internal energy to useful

work. In this regard, thermodynamics is more general than mechanics in its formulation of the law of conservation of energy. The energy forms that mechanics is concerned with are entirely convertible to work. Thermodynamics, on the other hand, considers the conversion of thermal energy to work, recognizing that only a fraction of the energy is convertible.

The principles that form the foundation of thermodynamics are embodied in several laws referred to as the *laws of thermodynamics*. In addition, *thermodynamic functions*, which interrelate the various properties of a system, are derived on the basis of these laws. A *system* refers to a part of space under consideration through whose boundaries energy in its different forms, as well as mass, may be transferred.

Within the context of its application to solving practical problems, thermodynamics is primarily concerned with systems at *equilibrium*. From an observational viewpoint, a system is at equilibrium if its properties do not change with time when it is isolated from its surroundings. The concept of equilibrium is a unifying principle that determines energy–work relationships as well as phase relationships.

The principles developed in Section 1.1 are fundamental in the sense that the system considered is not limited to any particular fluid type.

1.1.1 Laws of Thermodynamics

The *first law of thermodynamics* is a formulation of the principle of conservation of energy. It states that the increase in the internal energy of a system equals the heat absorbed by the system from its surroundings minus the work done by the system on its surroundings. For infinitesimal changes, the first law is expressed mathematically by the equation

$$dU = dQ - dW \tag{1.1}$$

where dU is the increase in internal energy, dQ is the heat absorbed, and dW is the work done by the system. The dimensional units of U, Q, and W are energy units.

The internal energy, U, is a basic property that represents the energy stored in a system. It is related to other properties such as work and heat. In an *adiabatic* process, for instance, where no heat crosses the system boundaries, the work done by the system equals the change in its internal energy. This follows from the first law by setting $dQ = 0$. In a process where no work is done by or on the system, $dW = 0$, and the change in internal energy equals the heat absorbed or rejected by the system. Heat is considered positive when absorbed by the system, and work is considered positive when done by the system on its surroundings.

The *second law of thermodynamics* relates to the availability of energy in a system for conversion to useful work. In order for a system to perform work, it must have the capacity for spontaneous change toward equilibrium. For instance, a system comprising a hot subsystem and a colder subsystem is capable of performing work as heat passes from the hot to the cold subsystem. Part of the heat is converted to work, while the rest is rejected to the cold subsystem.

The Carnot Engine

An example of a process that can deliver work by absorbing heat from a hot reservoir and rejecting heat to a cold reservoir is the Carnot engine. This is an idealized model consisting of a sequence of processes, each of which is assumed to be *reversible*. A reversible process is one that can be reversed by an infinitesimal change in the external conditions. For instance, in order to compress a gas reversibly, the external pressure at any moment should be $P + \Delta P$, where P is the gas pressure at that moment and ΔP is a small pressure increment. The reversible compression can be changed to a reversible expansion by changing the external pressure to $P - \Delta P$. A reversible process consists of steps in which the system is at equilibrium. In a reversible process there are no losses due to friction or other factors.

Assume that the system used to carry out the Carnot cycle is an amount of *ideal gas* contained in a cylinder fitted with a frictionless piston. The concept of an ideal gas is introduced in Section 1.2. Of consequence at this point is the premise that for an ideal gas the internal energy, U, is a function of temperature only. The Carnot cycle consists of reversible *isothermal* and *adiabatic* processes. An isothermal process is one in which the system temperature is kept constant. An adiabatic process requires that no heat be transferred between the system and its surroundings. The steps are as follows:

1. Reversible adiabatic compression in which the gas temperature changes from T_1, the temperature of the cold reservoir, to T_2, the temperature of the hot reservoir. Since this is an adiabatic process, $dQ = 0$, and, from the first law, $-dW = dU$. The work done on the gas in this step is, therefore,

$$-W_{12} = U_2 - U_1$$

   where U_1 and U_2 are the values of the internal energy at temperatures T_1 and T_2, respectively.
2. Reversible isothermal expansion at temperature T_2, in which an amount of heat, Q_2, is absorbed by the gas from the hot reservoir. For an ideal gas, $dU = 0$ at constant temperature. Therefore, the work done by the gas in this step is

$$W_2 = Q_2$$

3. Reversible adiabatic expansion in which the gas temperature changes from T_2 to T_1. As in step 1, the work done by the gas is

$$-W_{21} = U_1 - U_2$$

4. Reversible isothermal compression to the original state in which an amount of heat, Q_1, is rejected to the cold reservoir at constant temperature T_1. The work done on the system is

$$W_1 = -Q_1$$

The net work done by the system is the sum of the work associated with these steps:

$$W = U_2 - U_1 + U_1 - U_2 + Q_2 - Q_1$$

$$= Q_2 - Q_1$$

The Carnot efficiency is defined as

$$\eta = \frac{W}{Q_2} = \frac{Q_2 - Q_1}{Q_2}$$

The significance of the reversibility of the above processes is that at the end of the cycle the system is brought back to its starting point with no losses incurred due to friction or other causes. Thus, as the system temperature is restored to its starting point, T_1, its pressure is also restored to its starting level of P_1. If the processes are not reversible, additional work would have to be done on the system to bring the pressure back to P_1. The net work would be less than $Q_2 - Q_1$, and the efficiency would be lower than the Carnot efficiency.

It can be shown that the Carnot efficiency may also be expressed as

$$\eta = \frac{T_2 - T_1}{T_2}$$

where the temperatures are on the absolute scale. This is the maximum efficiency attainable by an engine operating between a hot and a cold reservoir. Although developed for an ideal gas model, the efficiency of an engine operating with any medium between temperatures T_1 and T_2 will never exceed the above value.

Entropy

The two equivalent expressions of the efficiency imply that

$$\frac{Q_1}{T_1} = -\frac{Q_2}{T_2} \quad \text{or} \quad \frac{Q_1}{T_1} + \frac{Q_2}{T_2} = 0$$

This equation states that the sum of the Q/T ratio along a Carnot cycle is 0. In general, any closed cycle, starting at some point and moving along reversible paths and returning to the starting point, can be represented by many small isothermal and adiabatic steps. The heat transferred in the adiabatic steps is, by definition, 0. For all the isotherms contained in the loop, the summation of the heat absorbed in each isotherm divided by its absolute temperature is 0:

$$\sum_i \left(Q_i/T_i\right) = 0$$

As the isotherms become infinitely small, the summation may be written as an integral over the closed reversible cycle:

$$\oint dQ/T = 0$$

If any two points A and B are chosen along the reversible cycle, the cycle may be broken into two reversible paths: 1 and 2. The closed cycle integral may be written as the sum of two integrals:

$$\oint \frac{dQ}{T} = \int_A^B \left(\frac{dQ}{T}\right)_1 + \int_B^A \left(\frac{dQ}{T}\right)_2 = 0$$

Subscripts 1 and 2 designate the integration paths. Reversing the integration limits and sign of the second integral, the above equation is rewritten as

$$\int_A^B \left(\frac{dQ}{T}\right)_1 = \int_A^B \left(\frac{dQ}{T}\right)_2$$

Thus, the value of the integral of dQ/T from point A to point B is independent of the path between A and B. A function S, the *entropy*, is now defined such that the change in its value from point A to point B is given by

$$S_B - S_A = \int_A^B \frac{dQ}{T}$$

Since the integral on the right-hand side is independent of the path as long as it is reversible, the change in entropy is independent of the path, and the entropy itself is a function of the thermodynamic coordinates of the system, such as its temperature and pressure. The above equation is next written for an infinitesimal change in entropy:

$$dS = dQ/T \tag{1.2}$$

where dQ is transferred reversibly. Equation 1.2 is a consequence of the second law of thermodynamics and is thus considered the mathematical formulation of this law.

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