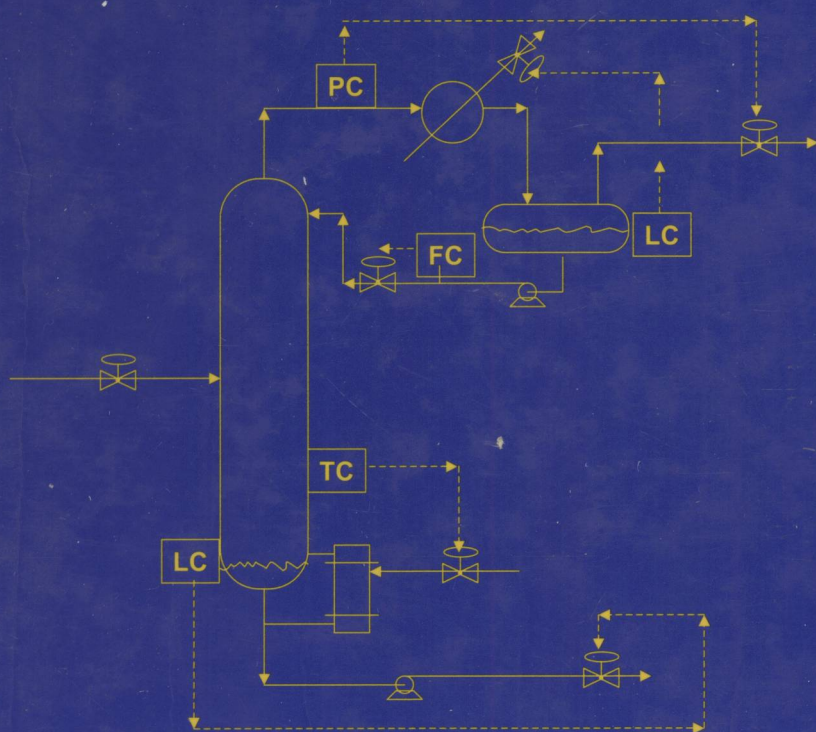


Distillation Design and Control Using AspenTM Simulation



WILLIAM L. LUYBEN

DISTILLATION DESIGN AND CONTROL USING ASPENTM SIMULATION

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Lehigh University
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AIChE[®]

 **WILEY-
INTERSCIENCE**

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DISTILLATION DESIGN AND CONTROL USING ASPENTM SIMULATION

*Dedicated to the memory of the pioneers of
Lehigh Chemical Engineering:
Alan Foust, Len Wenzel, and Curt Clump*

PREFACE

The rapid increase in the price of crude oil in recent years (as of 2005) and the resulting “sticker shock” at the gas pump have caused the scientific and engineering communities to finally understand that it is time for some reality checks on our priorities. Energy is the real problem that faces the world, and it will not be solved by the recent fads of biotechnology or nanotechnology. Energy consumption is the main producer of carbon dioxide, so it is directly linked with the problem of global warming.

A complete reassessment of our energy supply and consumption systems is required. Our terribly inefficient use of energy in all aspects of our modern society must be halted. We waste energy in our *transportation* system with poor-mileage SUVs and inadequate railroad systems. We waste energy in our *water* systems by using energy to produce potable water, and then flush most of it down the toilet. This loads up our *waste disposal* plants, which consume more energy. We waste energy in our *food* supply system by requiring large amounts of energy for fertilizer, herbicides, pesticides, tillage, and transporting and packaging our food for consumer convenience. The old farmers’ markets provided better food at lower cost and required much less energy.

One of the most important technologies in our energy supply system is distillation. Essentially all our transportation fuel goes through at least one distillation column on its way from crude oil to the gasoline pump. Large distillation columns called “pipestills” separate the crude into various petroleum fractions based on boiling points. Intermediate fractions go directly to gasoline. Heavy fractions are catalytically or thermally “cracked” to form more gasoline. Light fractions are combined to form more gasoline. Distillation is used in all of these operations.

Even when we begin to switch to renewable sources of energy such as biomass, the most likely transportation fuel will be methanol. The most likely process is the partial oxidation of biomass to produce synthesis gas (a mixture of hydrogen, carbon monoxide, and carbon dioxide) and the subsequent reaction of these components to produce methanol and water. Distillation to separate methanol from water is an important part of this process. Distillation is also used to produce the oxygen used in the partial oxidation reactor.

Therefore distillation is, and will remain in the twenty-first century, the premier separation method in the chemical and petroleum industries. Its importance is

unquestionable in helping to provide food, heat, shelter, clothing, and transportation in our modern society. It is involved in supplying much of our energy needs. The distillation columns in operation around the world number in the tens of thousands.

The analysis, design, operation, control, and optimization of distillation columns have been extensively studied for almost a century. Until the advent of computers, hand calculations and graphical methods were developed and widely applied in these studies. Since about 1950, analog and digital computer simulations have been used to solve many engineering problems. Distillation analysis involves iterative vapor–liquid phase equilibrium calculations and tray-to-tray component balances that are ideal for digital computation.

Initially most engineers wrote their own programs to solve both the nonlinear algebraic equations that describe the steady-state operation of a distillation column and the nonlinear ordinary differential equations that describe its dynamic behavior. Many chemical and petroleum companies developed their own in-house steady-state process simulation programs in which distillation was an important unit operation. Commercial *steady-state* simulators took over around the mid-1980s and now dominate the field.

Commercial *dynamic* simulators were developed quite a bit later. They had to wait for advancements in computer technology to provide the very fast computers required. The current state of the art is that both steady-state and dynamic simulations of distillation columns are widely used in industry and in universities.

My own technical experience has pretty much followed this history of distillation simulation. My practical experience started back in a high-school chemistry class in which we performed batch distillations. Next came an exposure to some distillation theory and running a pilot-scale batch distillation column as an undergraduate at Penn State, learning from Arthur Rose and “Black” Mike Cannon. Then there were 5 years of industrial experience in Exxon refineries as a technical service engineer on pipestills, vacuum columns, light-end units, and alkylation units, all of which used distillation extensively.

During this period the only use of computers that I was aware of was for solving linear programming problems associated with refinery planning and scheduling. It was not until returning to graduate school in 1960 that I personally started to use analog and digital computers. Bob Pigford taught us how to program a Bendix G12 digital computer, which used paper tape and had such limited memory that programs were severely restricted in length and memory requirements. Dave Lamb taught us analog simulation. Jack Gerster taught us distillation practice.

Next there were 4 years working in the Engineering Department of DuPont on process control problems, many of which involved distillation columns. Both analog and digital simulations were heavily used. A wealth of knowledge was available from a stable of outstanding engineers: Page Buckley, Joe Coughlin, J. B. Jones, Neal O’Brien, and Tom Keane, to mention only a few.

Finally, there have been over 35 years of teaching and research at Lehigh in which many undergraduate and graduate students have used simulations of distillation columns in isolation and in plantwide environments to learn basic distillation principles and to develop effective control structures for a variety of distillation column configurations. Both homegrown and commercial simulators have been used in graduate research and in the undergraduate senior design course.

The purpose of this book is to try to capture some of this extensive experience with distillation design and control so that it is available to students and young engineers

when they face problems with distillation columns. This book covers much more than just the mechanics of using a simulator. It uses simulation to guide in developing the optimum economic steady-state design of distillation systems, using simple and practical approaches. Then it uses simulation to develop effective control structures for dynamic control. Questions are addressed as to whether to use single-end control or dual-composition control, where to locate temperature control trays, and how excess degrees of freedom should be fixed.

There is no claim that the material is all new. The steady-state methods are discussed in most design textbooks. Most of the dynamic material is scattered around in a number of papers and books. What is claimed is that this book pulls this material together in a coordinated, easily accessible way. Another unique feature is the combination of design and control of distillation columns in a single book.

There are three steps in developing a process design. The first is “conceptual design,” in which simple approximate methods are used to develop a preliminary flowsheet. This step for distillation systems is covered very thoroughly in another textbook.¹ The next step is *preliminary design*, in which rigorous simulation methods are used to evaluate both steady-state and dynamic performance of the proposed flowsheet. The final step is “detailed design,” in which the hardware is specified in great detail, with specifics such as types of trays, number of sieve tray holes, feed and reflux piping, pumps, heat exchanger areas, and valve sizes. This book deals with the second stage, preliminary design.

The subject of distillation simulation is a very broad one, which would require many volumes to cover comprehensively. The resulting encyclopedia-like books would be too formidable for a beginning engineer to try to tackle. Therefore this book is restricted in its scope to only those aspects that I have found to be the most fundamental and the most useful. Only continuous distillation columns are considered. The area of batch distillation is very extensive and should be dealt with in another book. Only staged columns are considered. They have been successfully applied for many years. Rate-based models are fundamentally more rigorous, but they require that more parameters be known or estimated.

Only rigorous simulations are used in this book. The book by Doherty and Malone is highly recommended for a detailed coverage of approximate methods for conceptual steady-state design of distillation systems.

I hope that the reader finds this book useful and readable. It is a labor of love that is aimed at taking some of the mystery and magic out of designing and operating a distillation column.

WILLIAM L. LUYBEN

¹M. F. Doherty and M. F. Malone, *Conceptual Design of Distillation Systems*, McGraw-Hill, 2001.

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CHAPTER 1

FUNDAMENTALS OF VAPOR–LIQUID PHASE EQUILIBRIUM (VLE)

Distillation occupies a very important position in chemical engineering. Distillation and chemical reactors represent the backbone of what distinguishes chemical engineering from other engineering disciplines. Operations involving heat transfer and fluid mechanics are common to several disciplines. But distillation is uniquely under the purview of chemical engineers.

The basis of distillation is phase equilibrium, specifically, vapor–liquid (phase) equilibrium (VLE) and in some cases vapor–liquid–liquid (phase) equilibrium (VLLE). Distillation can effect a separation among chemical components only if the compositions of the vapor and liquid phases that are in phase equilibrium with each other are different. A reasonable understanding of VLE is essential for the analysis, design, and control of distillation columns.

The fundamentals of VLE are briefly reviewed in this chapter.

1.1 VAPOR PRESSURE

Vapor pressure is a physical property of a pure chemical component. It is the pressure that a pure component exerts at a given temperature when both liquid and vapor phases are present. Laboratory vapor pressure data, usually generated by chemists, are available for most of the chemical components of importance in industry.

Vapor pressure depends **only** on temperature. It does not depend on composition because it is a pure component property. This dependence is normally a strong one with an exponential increase in vapor pressure with increasing temperature. Figure 1.1 gives two typical vapor pressure curves, one for benzene and one for toluene. The natural log of the vapor pressures of the two components are plotted against the reciprocal of the

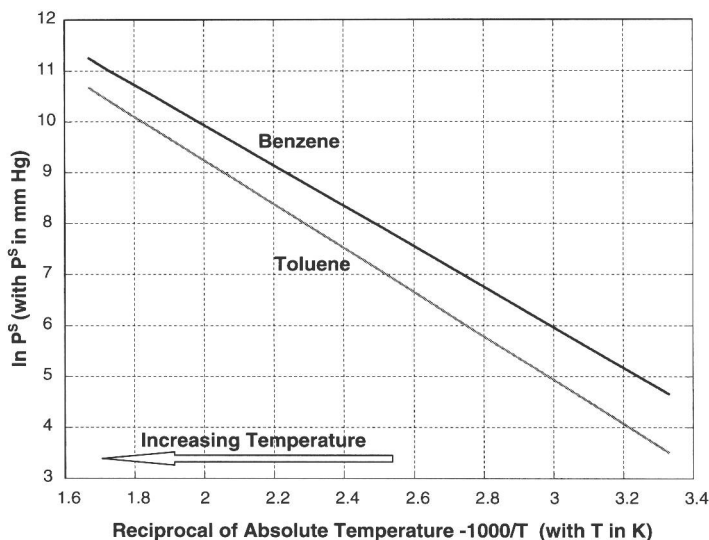


Figure 1.1 Vapor pressures of pure benzene and toluene.

absolute temperature. As temperature increases, we move to the left in the figure, which means a higher vapor pressure. In this particular figure, the vapor pressure P^S of each component is given in units of millimeters of mercury (mmHg). The temperature is given in Kelvin units.

Looking at a vertical constant-temperature line shows that benzene has a higher vapor pressure than does toluene at a given temperature. Therefore benzene is the “lighter” component from the standpoint of volatility (not density). Looking at a constant-pressure horizontal line shows that benzene boils at a lower temperature than does toluene. Therefore benzene is the “lower boiling” component. Note that the vapor pressure lines for benzene and toluene are fairly parallel. This means that the ratio of the vapor pressures does not change much with temperature (or pressure). As discussed in a later section, this means that the ease or difficulty of the benzene/toluene separation (the energy required to make a specified separation) does not change much with the operating pressure of the column. Other chemical components can have temperature dependences that are quite different.

If we have a vessel containing a mixture of these two components with liquid and vapor phases present, the concentration of benzene in the vapor phase will be higher than that in the liquid phase. The reverse is true for the heavier, higher-boiling toluene. Therefore benzene and toluene can be separated in a distillation column into an overhead distillate stream that is fairly pure benzene and a bottoms stream that is fairly pure toluene.

Equations can be fitted to the experimental vapor pressure data for each component using two, three, or more parameters. For example, the two-parameter version is

$$\ln P_j^S = C_j + D_j/T$$

The C_j and D_j are constants for each pure chemical component. Their numerical values depend on the units used for vapor pressure [mmHg, kPa, psia (pounds per square inch absolute), atm, etc.] and on the units used for temperature (K or °R).

1.2 BINARY VLE PHASE DIAGRAMS

Two types of vapor–liquid equilibrium diagrams are widely used to represent data for two-component (binary) systems. The first is a “temperature versus x and y ” diagram (Txy). The x term represents the liquid composition, usually expressed in terms of mole fraction. The y term represents the vapor composition. The second diagram is a plot of x versus y .

These types of diagrams are generated at a constant pressure. Since the pressure in a distillation column is relatively constant in most columns (the exception is vacuum distillation, in which the pressures at the top and bottom are significantly different in terms of absolute pressure level), a Txy diagram, and an xy diagram are convenient for the analysis of binary distillation systems.

Figure 1.2 gives the Txy diagram for the benzene/toluene system at a pressure of 1 atm. The abscissa shows the mole fraction of benzene; the ordinate, temperature. The lower curve is the “saturated liquid” line, which gives the mole fraction of benzene in the liquid phase x . The upper curve is the “saturated vapor” line, which gives the mole fraction of benzene in the vapor phase y . Drawing a horizontal line at some temperature and reading off the intersection of this line with the two curves give the compositions of the two phases. For example, at 370 K the value of x is 0.375 mole fraction benzene and the value of y is 0.586 mole fraction benzene. As expected, the vapor is richer in the lighter component.

At the leftmost point we have pure toluene (0 mole fraction benzene), so the boiling point of toluene at 1 atm can be read from the diagram (384.7 K). At the rightmost point we have pure benzene (1 mole fraction benzene), so the boiling point of benzene at 1 atm can be read from the diagram (353.0 K). In the region between the curves, there are two phases; in the region above the saturated vapor curve, there is only a single “superheated” vapor phase; in the region below the saturated liquid curve, there is only a single “subcooled” liquid phase.

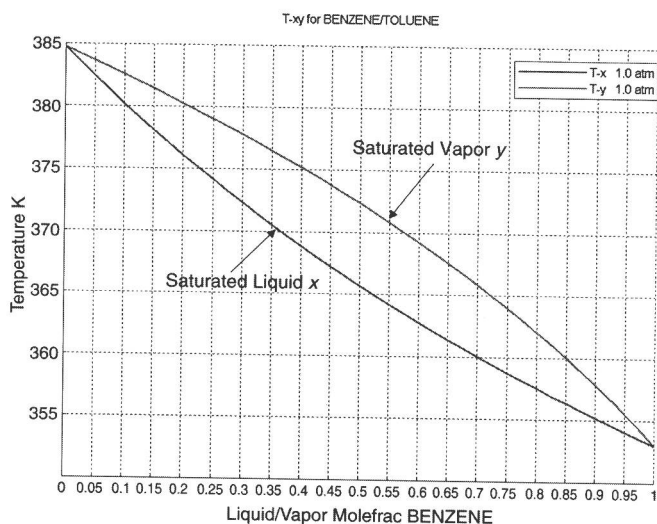


Figure 1.2 Txy diagram for benzene and toluene at 1 atm.

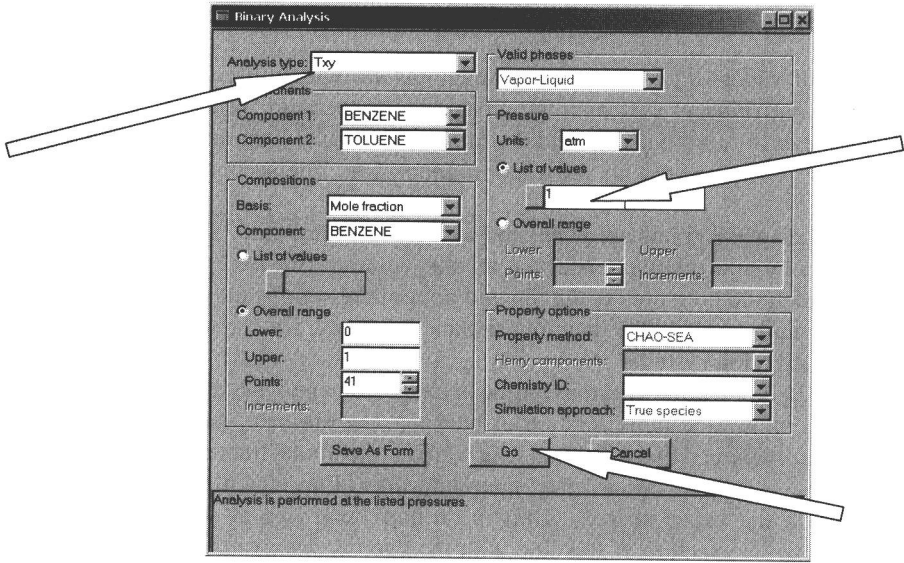


Figure 1.3 Specifying T_{xy} diagram parameters.

The diagram is easily generated in Aspen Plus by going to *Tools* on the upper toolbar and selecting *Analysis, Property, and Binary*. The window shown in Figure 1.3 opens and specifies the type of diagram and the pressure. Then we click the *Go* button.

The pressure in the T_{xy} diagram given in Figure 1.2 is 1 atm. Results at several pressures can also be generated as illustrated in Figure 1.4. The higher the pressure, the higher the temperatures.

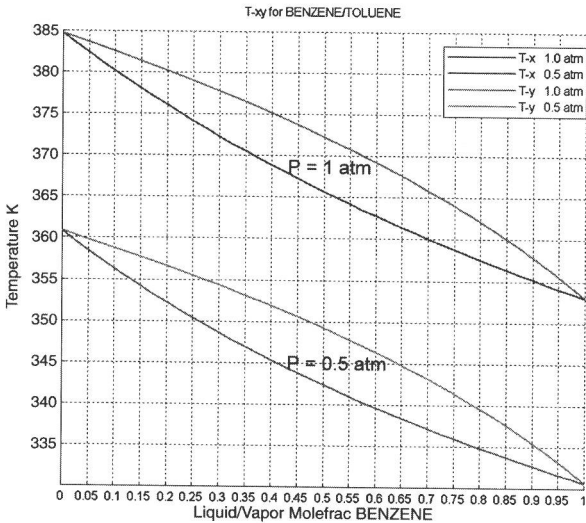


Figure 1.4 T_{xy} diagrams at two pressures.

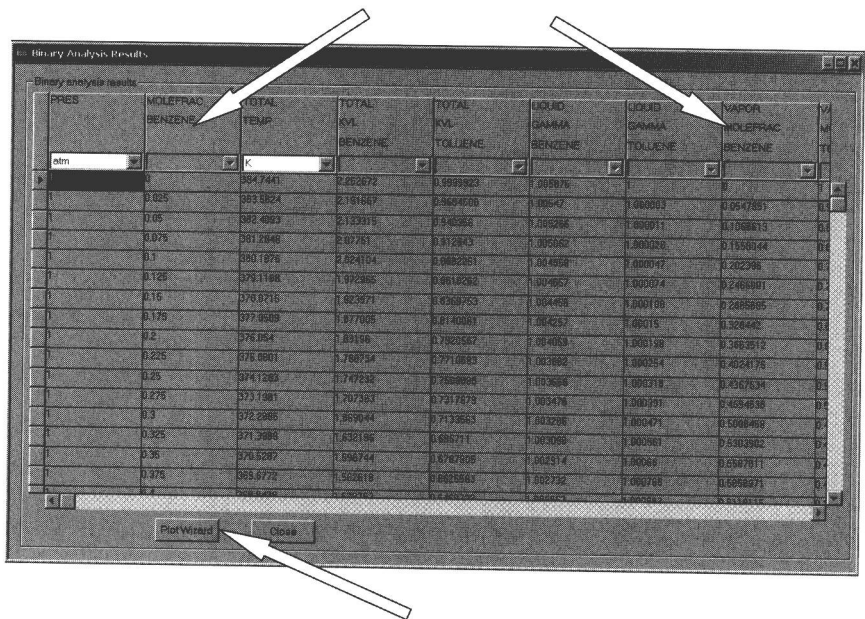


Figure 1.5 Using Plot Wizard to generate xy diagram.

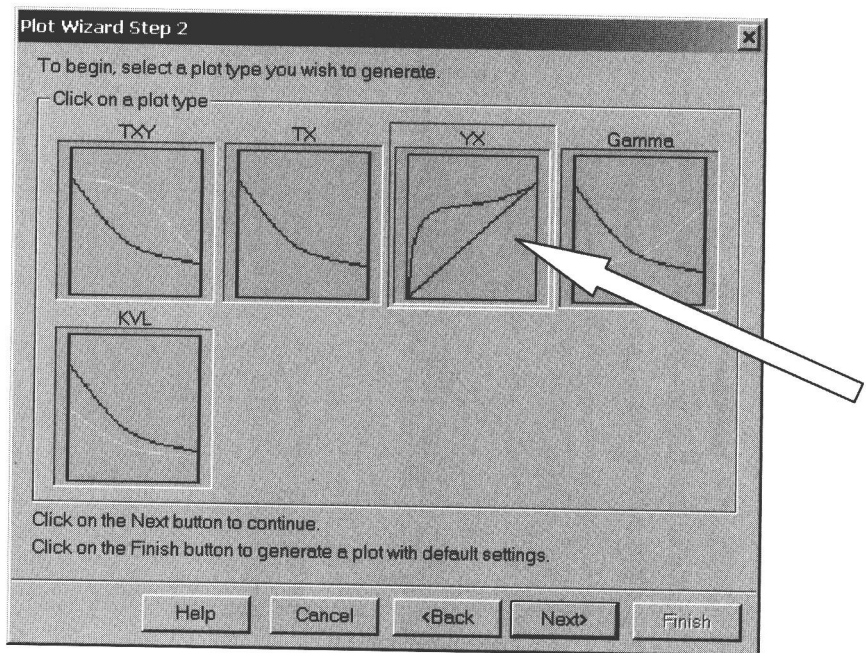


Figure 1.6 Using Plot Wizard to generate xy diagram.

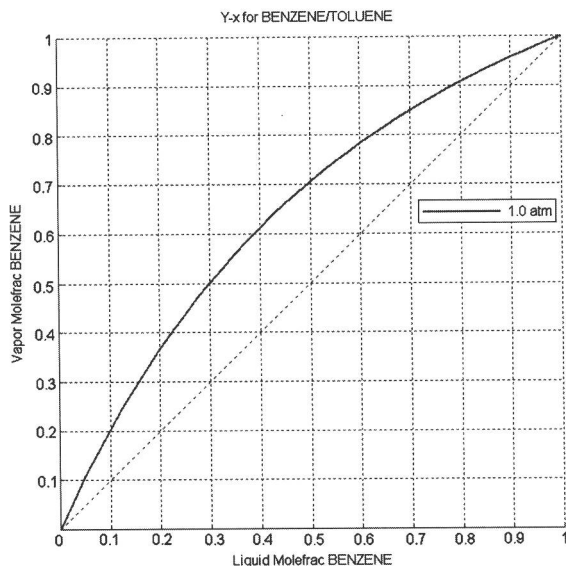


Figure 1.7 xy diagram for benzene/toluene.

The other type of diagram, an xy diagram, is generated in Aspen Plus by clicking the *Plot Wizard* button at the bottom of the *Binary Analysis Results* window that also opens when the *Go* button is clicked to generate the Txy diagram. As shown in Figure 1.5, this window also gives a table of detailed information. The window shown in Figure 1.6 opens, and *YX* picture is selected. Clicking the *Next* and *Finish* buttons generates the xy diagram shown in Figure 1.7.

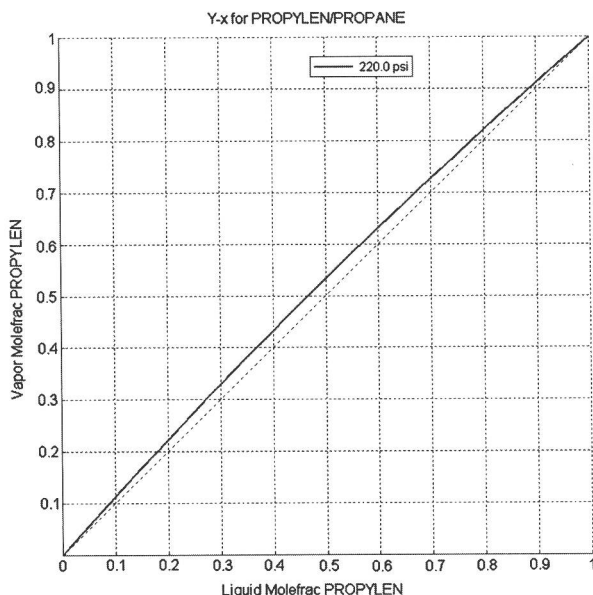


Figure 1.8 xy diagram for propylene/propane.