ChE classroom

TEACHING STAGED-PROCESS DESIGN THROUGH INTERACTIVE COMPUTER GRAPHICS

KENNETH R. JOLLS, MICHELLE NELSON, DEEPAK LUMBA
Iowa State University
Ames, IA 50011-2230

Graphical methods have long played a role in the teaching of separations processes. The classic papers of Ponchon,[1] Savarit,[2] and McCabe and Thiele[3] described graphical techniques for staged-distillation design that remain in use today more than half a century after their creation. Similar procedures are employed for absorption and extraction and for a number of the less frequently encountered processes.

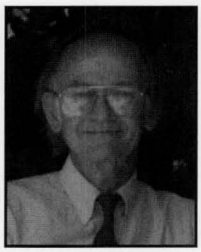
While such methods are useful pedagogically and their results more rapidly assimilated than those from numerically solved processes, they are also tedious, time-consuming, and require no small amount of drafting skill. Cumulative errors due to poorly constructed lines, missed intersections, and inaccurate interpolations can alter a drawing and mask the trends one wishes to show. Moreover, parametric cases are almost impossible to construct in any reasonable period of time. Thus the benefits of these visualized designs are too often overshadowed by the difficulties involved in producing them.

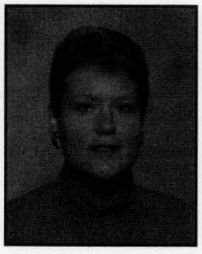
Several workers in recent years have used the computer to eliminate the tedium and inaccuracy of manual graphic design. Gaskill[4] used an analog-logic computer in rep-op mode to produce McCabe-Thiele displays for systems at constant relative volatility. His examples showed variations in all of the usual operating parameters as well as misplacement of the feed tray. Calo and Andres[5] employed Smoker's method for constant-α distillations having both multiple feeds and multiple side-draws. Their program was interactive and yielded expandable McCabe-Thiele plots on a storage CRT.

Working in Cornell University's Computer-Aided Design and Instructional Facility, Golnaraghi *et al.*[6] used vector-refresh graphics to produce McCabe-Thiele diagrams on an Evans and Sutherland Multipicture System. Their scheme provided for rapid data input and recomputation of parametric cases through a stylus-tablet arrangement. More recently, Kooijman and Taylor[7] have used graphics to accompany their ChemSep program, and Fogler and Montgomery[8] have created a variety of separations modules with associated visuals.

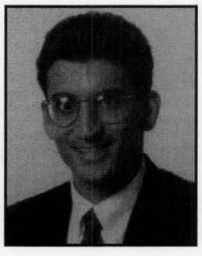
At Iowa State we have developed a method that applies computer graphics to the three major separations procedures and to several process types within each. Using the FLOWTRAN simulator[9] to solve the balance and thermodynamic equations for each operation, we have written pre- and post-processing software to simplify data entry and to

Kenneth R. Jolls *has undergraduate degrees from Duke and North Carolina State Universities and graduate degrees from the University of Illinois. His specialties include applied electronic instrumentation, thermodynamics, and computer visualization in chemical engineering research and practice. He was formerly on the faculty at the Polytechnic Institute of Brooklyn and has had sabbatical leaves at U.C. Berkeley and at Cornell.*





Michelle Nelson *(now Fendrich) received her BS and MS degrees in chemical engineering from Iowa State University. She is employed as a thermal engineer at Commonwealth Edison's nuclear power plant at Morris, Illinois, where she is currently working on heat-rate improvement.*



Deepak Lumba *is a Senior Project Engineer in the Applications Research and Development Group of Praxair, Inc., Tarrytown, New York. He is presently developing new applications for industrial gases in the chemical industry. He holds a BTech in chemical engineering from the Indian Institute of Technology, Kharagpur, India, and the MS and PhD degrees from Iowa State University.*

display the numerical results of the simulations in a variety of standard formats. For single-solute absorption and stripping, for extraction with and without reflux, and for several configurations of binary distillation, our program allows for interactive building of input files, execution of the FLOWTRAN runs, and display of the computed results using medium-resolution color-graphics devices. Auxiliary COST blocks are combined with the FLOWTRAN separations blocks ABSBR, EXTRC, FRAKB, AFRAC, IFLSH, and BFLSH to retrieve the computed stream properties and store the data in display files. After each simulation run a menu of graphical options lists the displays available for the particular process involved.

Our program is called "Simulation Graphics," and it provides all computing support for the undergraduate mass-transfer course at Iowa State. Working in small groups, students use the program to generate graphical solutions to problems involving the three separations processes noted above. During a typical term, five such problems are assigned, one each in absorption and extraction and three in distillation. The problems are worded so as to correlate with the current course textbook (Treybal[10]), and each problem concludes with a process specification for which an optimum design must be found.

To use the program, students choose the process, indicate the run conditions (feed properties, number of stages, reflux ratio, etc.), execute the FLOWTRAN simulation, and then select the type of display that they wish to see. For distillation they can view either Ponchon-Savarit or McCabe-Thiele plots, an overall block diagram or the stage-by-stage details for selected regions of the tower, or other diagrams showing zoomed displays, logarithmic plots of concentration, and T-x-y functions. Primary viewing is on a video terminal, but hard copies may be made when needed.

The power of the technique lies in its speed and its graphical and chemical accuracy. Running on an unencumbered VAX 11/780 computer, a simulation may be specified, executed, and its results displayed in about sixty seconds. Repetitions that involve changing only one or two input variables may require half that time. For absorption and stripping, students can explore a range of L/G ratios, inefficient stages, heat addition or removal, side streams, and other related changes. Extraction variants include solvent purity, S/F ratio, and refluxed vs. nonrefluxed operation. Moreover, these changes can be viewed in time spans short enough to give continuity to the learning process. Manual methods, especially when executed carefully, are far too slow to be effective vehicles for showing trends.

Visual accuracy is guaranteed by the direct plotting of computed results onto medium-resolution graphics devices. While the program currently produces displays on Tektronix hardware, we plan ultimately to port it to other systems of comparable graphic quality (EGA-equipped PCs, DEC stations with color graphics, etc.). Color is an important attribute in this method because it distinguishes the various components of a staged-process display—equilibrium and operating curves, rays, feed and product lines—and also clarifies the accompanying text that reports the numerical results for each run.

. . . we have developed a method that applies computer graphics to the three major separations procedures and to several process types within each. Using the FLOWTRAN simulator[9] to solve the balance and thermodynamic equations for each operation, we have written pre- and post-processing software to simplify data entry and to display the numerical results of the simulations in a variety of standard formats.

Chemical accuracy follows from the way in which phase-equilibrium data are entered. As with other process simulators, FLOWTRAN contains a data-regression utility (VLE) that accepts data in various formats and generates best-fit activity-coefficient parameters based on user-specified thermodynamic models. Various options are available for vapor pressure, fugacity, activity coefficients, liquid density, and the like. The procedure is simple and fast and guarantees that subsequent operations performed on a system are based on a realistic equilibrium function. The repeated assumption of ideality, as is often the practice when teaching basic separations techniques, sends students the wrong message about the value of chemical accuracy. Using VLE we have successfully modeled nonideal and azeotropic vapor-liquid systems for distillation as well as partially miscible liquid-liquid equilibria for extraction.

In designing this software we have attempted to give graphical support to many of the process variants that can be handled by FLOWTRAN. Dual feeds, side streams, tray heaters and coolers, inefficient stages, and partial condensers can not only be simulated but will also be represented in the computer-generated displays through the correct graphical constructions. Alternate graphical modes involving zoomed and logarithmic plots and displays of the stream details for adjacent trays provide complete definition of a process and allow for verification of energy and material balances and physical-property relationships.

CLASSROOM USE

Graphical design for staged processes is traditionally carried out *before the fact.* Diagrams are constructed to deter-

mine the operating conditions for a process—number of trays, L/G radio, heating and cooling loads, and other parameters that specify the operation. "Simulation Graphics" provides *after-the-fact* information. Conditions are supplied to the simulator, and if the separation is successful the results may then be plotted in any of the standard forms. While traditional methods *yield* the number of stages needed for a separation, simulators *require* such numbers before runs can be made. Manual methods set reflux and L/G ratios on the basis of predetermined limits. "Simulation Graphics" must be given those ratios before it can run.

This subtle but important distinction influences the way that this software is used in the classroom. Our assignments always begin with cases that work—sets of operating conditions that cause FLOWTRAN to converge the balances, effect a solution, and build a display file for subsequent plotting. Variations are then imposed upon these base cases to achieve the actual operations desired.

We feel that there is little pedagogical loss in this approach. The advantages gained from students being able to introduce process variations quickly, easily, and with full graphical support far outweigh any effort required by a shift in teaching style. With this software we have been able to assign problems of greater significance, having more complexity, requiring less student effort, and offering a higher expectation of performance than was possible with classical methods. Moreover, it exposes our students to the benefits of computer-based visualization early in their development and in a context uniquely associated with chemical engineering.

Students learn to use "Simulation Graphics" quickly. Each group has an introductory session with the instructor before running the first (absorption) assignment. Handout materials lead the students through the procedure and complement the prompts that appear on the screen. Learning the operations for the distillation and extraction problems that come later in the course requires only a small additional effort.

In the remainder of this paper we will show selected displays from among those generated in our current group of assignments. The figures were produced with a Tektronix model 4696 printer with all colors set to dark blue for maximum contrast. Where information has been lost because of the absence of color, callouts have been added for clarity.

GAS ABSORPTION

Figure 1 shows the mole-fraction-based equilibrium curve and operating line for the removal of dilute (1.0%) benzene vapor from nitrogen using n-hexadecane as the absorbing liquid.* Seven equilibrium trays are used with a liquid/gas ratio of 0.22 (L_s/G_s is the solute-free ratio). A regular solution model yielded the near-Henry's law equilibrium curve, and the small amount of solute transferred accounts for the limited temperature increase and the straight operating line on fraction coordinates.

** The oasic FLOWTRAN data base contains physical properties for 180 compounds, but it may be expanded at will using information from standard sources.*

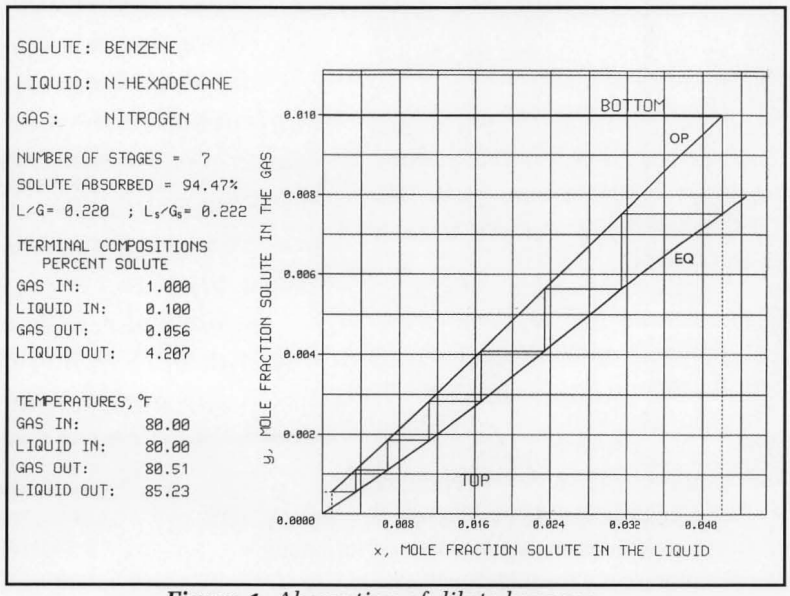


Figure 1. *Absorption of dilute benzene.*

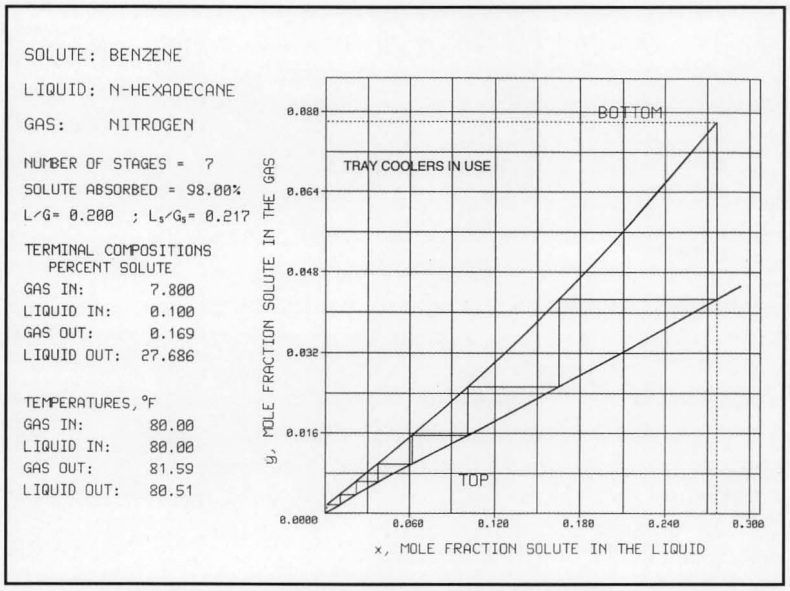


Figure 2. *Absorption of concentrated benzene.*

Students learn to use "Simulation Graphics" quickly. Each group has an introductory session with the instructor before running the first (absorption) assignment. Handout materials lead the students through the procedure and complement the prompts that appear on the screen.

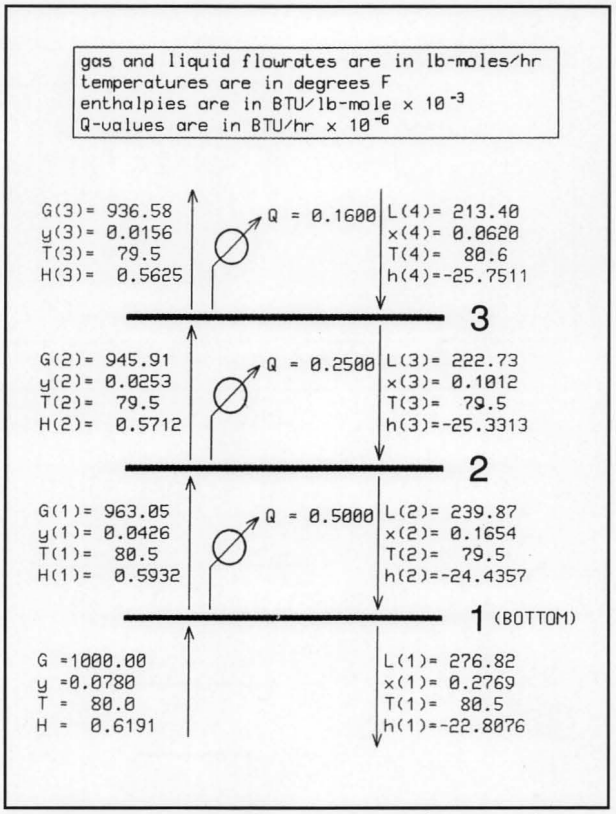


Figure 3. *Heat removal using tray coolers (x, y denotes mole-fraction benzene).*

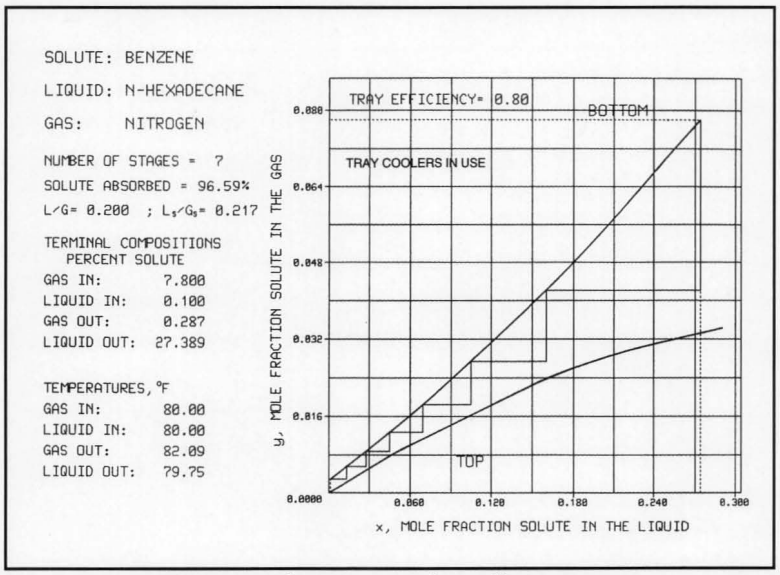


Figure 4. *Absorption with inefficient trays.*

Figure 2 shows the same process but with a more concentrated benzene mixture (7.8%) and a correspondingly curved operating line (range scaling is automatic). The temperature rise and reduced solubility that one would normally expect from the greater heat release has been counteracted with coolers on the lower five trays. Heat withdrawals were adjusted manually for near-isothermal operation.

An alternate display mode is shown in Figure 3, where the stream details are given for the three trays at the bottom of the column. In this mode, one selects a tray and the program responds with the flowrates, concentrations, temperatures, enthalpies, and other details for the specified tray (number two in this case) and for those immediately adjacent. Symbols for the coolers are shown along with the quantities of heat removed.

Figure 4 shows the results from a third absorption run where a Murphree gas efficiency of 0.8 was applied uniformly to all trays and the temperature variation was again suppressed with coolers. Points for the normal equilibrium curve are back-calculated from the nonequilibrium results and the specified E_{MG}.

Students are asked also to vary the number of contacts and the liquid and gas flowrates in this example so as to produce a near-pinch at the top of the column. A separate option gives the limiting L/G ratio that applies for given operating conditions. Such parametric cases may be run in quick succession to produce multiple results that aid the perception of trends.

For processes of absorption and stripping involving straight lines (dilute solutions, near-isothermal operation, mole-ratio analysis, etc.), students are asked to compare the rigorous simulator results to those predicted by the Kremser equation[11] for the same sets of terminal conditions. While verifying a useful tool for approximate analysis, this exercise also promotes confidence in the notion of linearizing a separations process for rapid modeling. Wankat[12] discusses this technique at length.

BINARY DISTILLATION

Constant-pressure distillation of two feeds in the system acetone-isopropanol is shown in Figures 5-7. A "title page" (not shown) presents the overall process and shows heating and cooling loads and terminal flowrates, compositions, and temperatures. The McCabe-Thiele plot in Figure 5 shows the relative constancy of the liquid/vapor ratios in the

column and also the thermal conditions and (optimum) entry-points for the two-phase feeds.* Nonequilibrium trays may be specified as an option.

The Ponchon-Savarit diagram in Figure 6 adds thermal information and permits confirmation of the difference points for the three sections of the tower. (Individual feed conditions are shown by the square symbols.) Students mount these plots on large, identically ruled graph sheets and extend the truncated rays to their intersections at the actual Δ points. Heat duties are noted in both the accompanying text and also in the stage details for the top and bottom sections of the tower. (The latter appears in Figure 7.)

For simplicity, pressure in this problem was held constant at one atmosphere throughout the column. A linear pressure profile may also be imposed by setting the pressures for the top and bottom trays to suitably spaced values. Effluent compositions from each tray are then determined from the local pressure value and the physical-property model in effect. The property model in the example shown here comprised Antoine vapor pressures, Redlich-Kwong vapor and liquid fugacities (the latter Poynting-corrected), and Van Laar activity coefficients evaluated so as to minimize K-value error between experimental and predicted data.[13]

The concept of entropy increase on mixing may also be illustrated in this problem by having students combine the two feeds and distill the composite in a separate, single-feed column. The (adiabatically) combined feed-state lies on the line connecting the individual feeds in Figure 6 and is shown by the diamond symbol. With other variables held constant, the reflux is increased until the purity of

*"*McCabe-Thiele*" is a generic name for this diagram. The operating lines connect* rigorously *determined stream compositions and are straight only if the L/G ratios do not vary. Similar comments also apply to the q-line construction.*

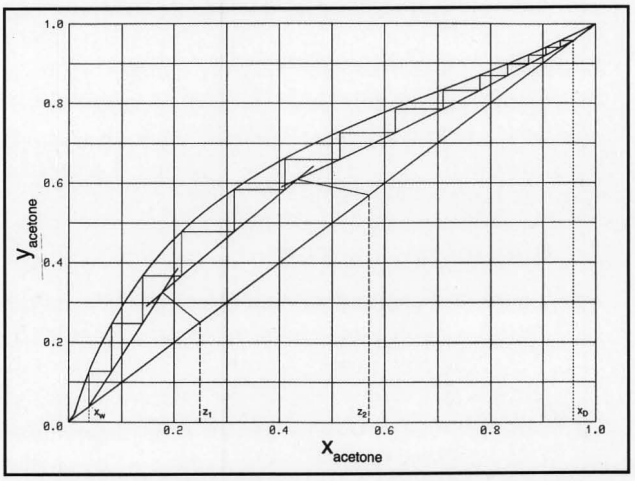


Figure 5. *Acetone-isopropanol distillation, McCabe-Thiele analysis*

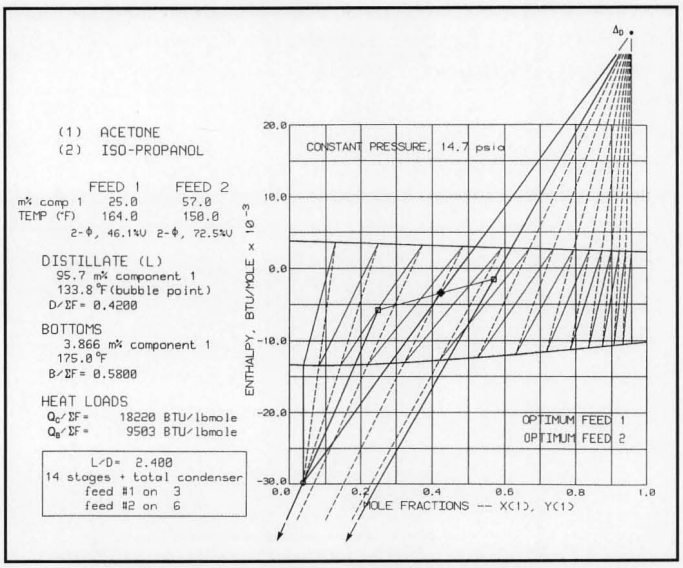


Figure 6. *Distillation with two feeds.*

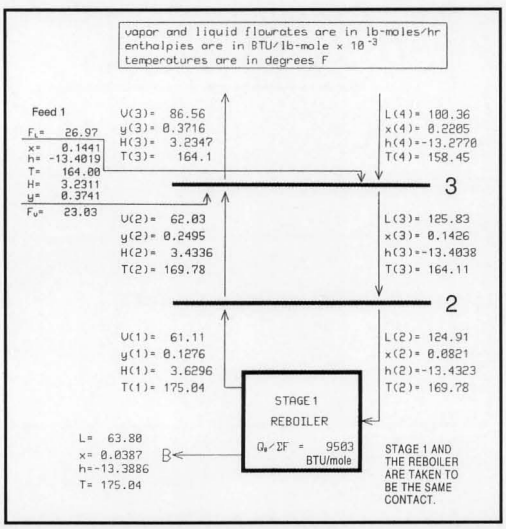


Figure 7. *Lower stages and (partial) reboiler.*

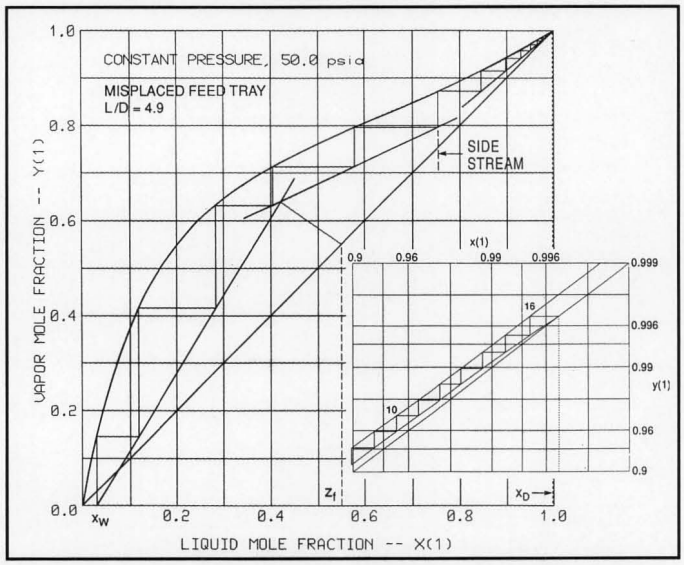


Figure 8. *Open-steam distillation of methanol (1) - water (2).*

the single-feed distillate matches that obtained when the feeds are separated. The added heat load is then related qualitatively to the energy needed to "demix" the composite (approximately a 20% increase in this example).

Figure 8 shows the results of open-steam distillation of a two-phase feed in the methanol-water system. Wet steam at 50 psia and 10% moisture is fed to the bottom of a 16-tray tower with the feed nozzle at tray 3 and a side-stream port (for liquid withdrawal) at tray 6. The McCabe-Thiele diagram shows the large concentration-change-per-stage in the stripping section, the misplaced feed condition, and the high-purity distillate (x_D=0.9968). The rectifying line is broken at tray 6 to reflect the withdrawal of 40% of the liquid flow. The accompanying numerical data (not shown here) report the condenser duty and the conditions of the entering steam to give the energy and cooling requirements for the process.

Tray compositions at the top of the tower are given by a separate logarithmic plot (seen here as an inset to Figure 8). High-purity bottoms products may also be represented in this way.

SOLVENT EXTRACTION

As a final example, pure isopropyl ether is used to separate acetic acid from aqueous solution in a countercurrent extractor with four perfect stages. Isothermal conditions are assumed. Phase-equilibrium data were obtained for the acetic acid-water-ether ternary,[10, p. 494] and Renon activity coefficients were fitted to the experimental coexistence curve to include acid compositions well in excess of those involved in the extraction.

Figure 9 shows the right-triangular diagram for the process. The bulk-mixing point (□) reflects the mass balance among the terminal streams, and the position of the difference point gives a solvent-to-feed ratio approximately 2.7 times the minimum.

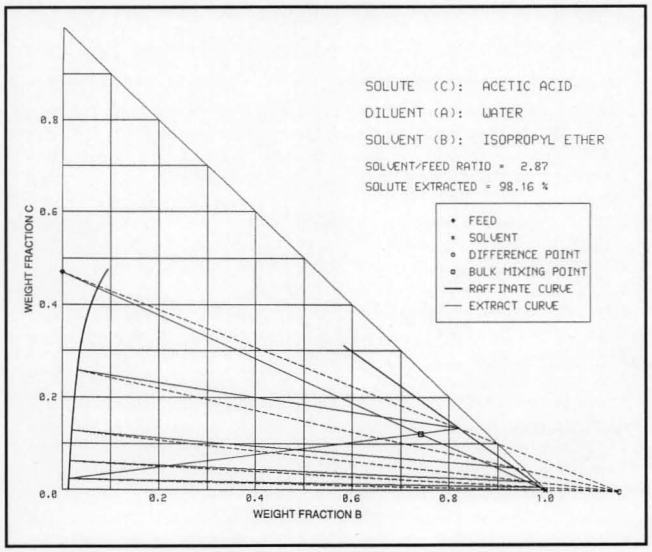


Figure 9. *Liquid-liquid extraction.*

The same information may be plotted on solute-distribution coordinates, where raffinate/extract flow ratios may be obtained from the local slope of the operating curve (or from the actual flows given on the plots of individual stages). Other display modes include coordinates for solvent-free and immiscible-liquid flows, as well as for the basic ternary phase diagram.

IN SUMMARY

For each of the above processes, the FLOWTRAN block diagram is constructed by "Simulation Graphics" instead of by the user. Two-feed distillation uses the FLOWTRAN unit FRAKB in a normal configuration—the feed conditions, the fraction overhead, the reflux, and the number of trays of specified efficiency determine the rates and compositions of the products. The open-steam example employs the block AFRAC, but in a less conventional mode, where internal control loops yield an effective total condenser and a reflux-dependent product. But these connections are unseen by the user who specifies the process by responding to separations-language prompts and is thus shielded from detailed interaction with the simulator.

Graphical operations in the program are independent of the simulations. All numerical results are written to display files which are used separately to produce the various drawings available. The usual FLOWTRAN output files (histories, FTO files, etc.) are turned off during normal operation but may be re-enabled within the program for purposes of debugging.

"Simulation Graphics" will continue to grow as we add more algorithms to assemble the FLOWTRAN blocks in new and more varied ways. The principal efforts at present involve creating interactive access to the FLOWTRAN physical-property base and employing additional control loops to expand the ways in which processes may be specified.[14] Inclusion of the data-regression utility within the interactive shell is also planned.

Future enhancements will include utilities to model continuous-contact processes and also expanded graphics capabilities for representing various aspects of multicomponent separations. Extensions to other process simulators and to other computing systems are likewise being considered.

Our goal in developing this software has been to create a precise pedagogical tool, undiluted by limitations and simplifying assumptions, yet fast and easy enough to use for a typical undergraduate separations course. Computer-assisted instruction should *broaden* a student's experience, first by removing the tedium of repetitive and mechanical operations and second by filling the time saved with work that

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expands his or her understanding of the subject. "Simulation Graphics" does both. Not only are the tedious details of manual graphic design eliminated, but also the scope of assignable problems is greatly increased, even to include open-ended examples where students must search through many solutions to satisfy a constraint or find some optimum.

An advantage also arises from exposing students to computer-based visualization. Chemical engineering has moved less rapidly than other engineering fields to capitalize on the enormous conceptual boost offered by visual thinking—particularly in the classroom.[15] Visualization models abound in thermodynamics, in transport phenomena, in reactor design, and in other core areas of the discipline.[16-18] This application to graphical models of staged processes is a natural and significant step toward accelerating that movement.

A CLOSING NOTE

Over seventy years ago, Marcel Ponchon[1] described his graphical method for binary distillation design. His introductory remarks, translated in part below, are as valid today as they were then. The efforts reported here and by those working before us have attempted to make those ideas more accessible through modern computer graphics.

> *The theory of distillation columns is rather complex, requiring long and difficult calculations. But it is possible, without going into the theory, to replace those calculations with graphical constructions that permit the solution of a rather large number of problems.*

ACKNOWLEDGMENTS

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BOOK REVIEW: Networking

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presented conceptual frameworks that help the reader to grasp *why* NETWORKING is so vital in today's rapidly changing and diverse environment, *what* needs to be done to be an effective NETWORKER, and *how* to develop their own NETWORKING prowess.

Many of the NETWORKING principles can come fairly easily to gregarious, highly self-motivated and self-confident people. However, for the other (~) 95% of us, the idea of initiating contact with friends, neighbors, friends of friends—*perfect strangers!*—can be intimidating to the point of paralysis! This book can help anyone muster the courage and conviction to become an effective NETWORKER.

Some people will prefer to work through this book on their own. Others will realize greater benefit by working with a partner or in groups (*e.g.,* AIChE). The reader should have time to contemplate many of the ideas presented and to complete the recommended assignments in order to maximize full learning potential. Dialog, discussion, and sharing ideas with others should also prove beneficial.

In summary, NETWORKING is an important life skill for all of us. This book will prove very valuable to everyone who reads it. It should be required by those responsible for educating young people who are preparing to enter the professional world. ❐