THE USE OF COMPUTER GRAPHICS TO TEACH THERMODYNAMIC PHASE DIAGRAMS

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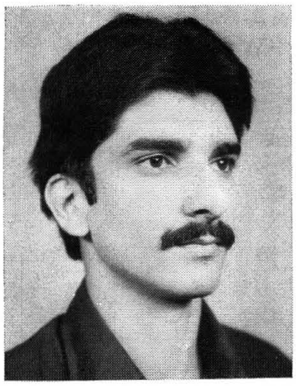
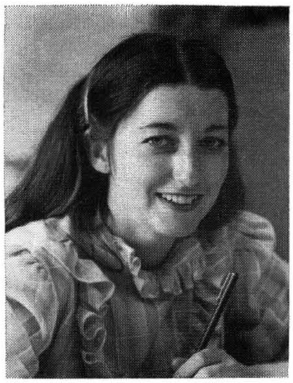
THE TEACHING of thermodynamic phase diagrams poses problems which affect both the instructor and the students. The usual approach in which the three-dimensional pressure-temperature-composition diagrams for binary fluid mixtures are represented on a two-dimensional page is difficult for students to visualize. Traditionally, in order to simplify this complex situation, 'cuts' at constant pressure, temperature, or composition are made to show a truly two-dimensional diagram describing the relationship between two of the three independent variables. However, the inter-relationship of all the variables involved is lost with this approach, and the problem of comprehension intensifies as the complexity of the phase behavior increases. Construction of three-dimensional models offers an alternative solution, but they are difficult and time-consuming to produce and offer no possibility for student interaction.

At Cornell an alternative to traditional approaches was sought to improve the quality of teaching and the level of comprehension of the students. Computer graphics offers an innovative solution to these difficulties: present-day graphics hardware can perform rotational transformations of three-dimensional images almost instantaneously and allows extensive manipulation of the viewed image by the user, making this an extremely powerful tool eminently suited to the task at hand. During the past two years a highly interactive "user friendly" graphics package has been developed depicting the three-dimensional phase behavior of binary fluid mixtures, and it has been used in both undergraduate and graduate courses with great success.

THE GRAPHICS WORKSTATION

The Computer Aided Design Instructional





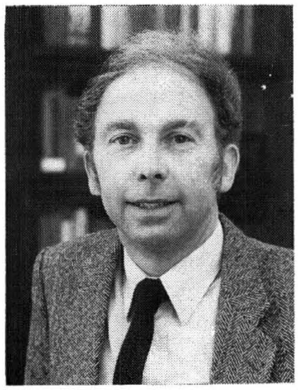


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FIGURE 1. An example of a typical workstation showing the Evans and Sutherland vector refresh graphics monitor with VT100 terminal, electronic tablet and stylus.

Facility (CADIF) at Cornell houses "state-of-the-art" computer graphics equipment used solely for teaching (and developmental work towards education). The central computers for the facility are Digital Equipment Corporation (DEC) VAX machines, an 11/780 and an 11/750, running the VMS operating system, with DEC PDP 11/44 machines as post-processors. Attached to these machines are two different types of graphical display equipment for student use: vector refresh stations with dynamic three-dimensional capabilities and color raster stations for applications requiring color. In this application, the vector refresh workstations were used exclusively, these being the highly sophisticated Evans and Sutherland Multipicture Systems. Each workstation has a digitizing tablet and electronic stylus as the primary input peripheral for cursor control, with a DEC VT100 terminal for alphanumeric input. A typical workstation is shown in Fig. 1. An electrostatic plotter is also available for hardcopy output, a useful and necessary addition allowing students to submit a record of their progress to the instructor.

The software, which is the heart (or perhaps more appropriately, the brains) of this application, was written in FORTRAN making use of system graphics software routines developed at CADIF. The consideration of ergonomic factors to produce a well designed application in terms of its "user-friendliness" was considered essential to promote ease and clarity of use of the graphics package as well as increased flexibility. Some of the ways this was achieved include the following points: extensive 'help' messages and prompts for required input were made available, clear consistent "menus" for optional choices of interactive response by the program were produced, and the ability to recover from mistakes or unintentional "miskeying" was provided. It was an original tenet of this study that students should not have to read a computer manual before using the programs. The emphasis is thus on learning engineering principles without requiring prior expertise in computing.

REPRESENTATION OF THE PHASE DIAGRAMS

The phase equilibrium data for binary mixtures needed for the representation of the phase diagram (i.e. pressures, temperatures and compositions) were generated using a theoretical model. The original Redlich-Kwong equation of state was employed for this purpose, chiefly because of the simplicity of its representation (since only two adjustable parameters are involved) and the reasonably realistic description of binary phase behavior it provides. This approach was also used by Willers and Jolls [1] who produced three-dimensional phase diagrams on a Cal Comp plotter using the same equation of state.

It has proven to be extremely popular with the students, and has raised the level of comprehension of this potentially difficult subject above that achieved previously by using conventional means.

The well-known Redlich-Kwong expressions describing the conditions for vapor-liquid or liquid-liquid equilibrium in terms of the pressures and chemical potentials of both phases were used to generate data points P, T, V_L, V_G, x_1, and y_1 covering a region from the higher of the pure component triple points to a temperature above both critical temperatures. The nonlinear equations involved were solved using a multidimensional Newton-Raphson [2] technique. Close to the critical region, however, convergence problems were encountered which were due, we believe, to singularities in the Jacobian matrix. These difficulties were overcome by using the Marquardt [3] method which combines the advantages of Newton-Raphson and Steepest Descent algorithms. Here Argonne National Laboratory's 'MINPAK'

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software package provided the subroutine for a Marquardt method of solution. Solving for vapor-liquid critical lines also provided a challenge. Neither of the previous techniques mentioned was able to reproduce these highly non-linear equations, and a specialized algorithm due to Deiters [4] was employed for their solution.

Scott and Van Koynenburg [5, 6] classified the experimentally observed types of fluid phase diagrams into six classes, based on the presence or absence of three-phase lines and their connection with the critical lines. So far we have been able to cover the two simplest classes, I and II, although extension of the programs to cover the other classes is well underway. These more complex systems will provide an even more striking visual illustration of the advantage of using computer graphics. In classes I and II both components have similar critical temperatures with the vapor-liquid critical line passing continuously between them. In class II, however, the mixture is more non-ideal and exhibits liquid-liquid immiscibility at low temperatures. For this class, in addition to the vapor-liquid region encountered for class I, two other regions exist in the phase diagram, those of liquid-liquid equilibrium and a three-phase liquid-

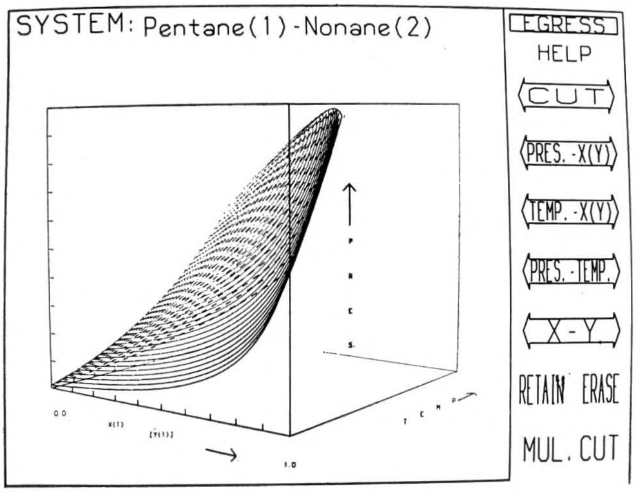

FIGURE 2. Three-dimensional phase diagram for a typical class I system, pentane-nonane. The solid and dashed lines show the vapor and liquid boundaries, respectively.

TABLE 1
Examples of Classes I- and II- Type Behavior Available for Display By the User

Binary Mixture	Azeotrope†	Temp Range K‡	Pressure Range Bars‡
	CLASS I		
Pentane-Nonane	N	425-590(594)	2.38-24.30(33.7)
Cyclopentane-Nonane	N	425-590(596)	2.39-21.92(45.2)
Pentane-Ethylbenzene	N	425-615(617)	4.18-36.70(37.4)
Acetone-Trichloromethane	Y−	420-530(535)	11.86-51.18(55.6)
	CLASS II		
Methane-Tetrafluoromethane	N	80-224.5(228)	1.25×10^{-4}-38.76(46.0)
Perfluoropentane-Pentane	Y,Het + Hom	240-505(506)	4.18×10^{-2}-39.28(39.7)

†N,Y = no, yes; + − = positive or negative deviation from Raoult's law; Het, Hom = heterogeneous, homogeneous azeotrope.

‡The figures in parentheses are the highest values of T_c and P_c occurring along the critical line.

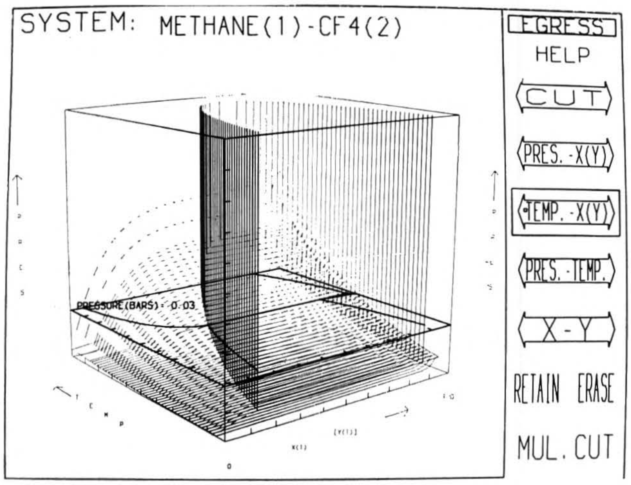

FIGURE 3. P-T-x diagram for the class II system, methane-tetrafluoromethane, showing the coexisting vapor-liquid equilibria (solid lines for the vapor, dashed for the liquid) and the region of liquid-liquid immiscibility (shown as solid vertical lines). Superimposed on the diagram (shown in bold) is a T-x cut at a pressure of 0.03 bars.

liquid-gas line. Examples of the binary systems chosen to illustrate the phase behavior of classes I and II are shown in Table 1. Some of the available systems exhibit azeotropic phenomena with either positive or negative deviations from Raoult's Law, and of either a heterogeneous or homogeneous nature. Photographs depicting some of the computer-generated phase diagrams are reproduced in Figures 2-6 illustrating the kind of image displayed for the user to manipulate.

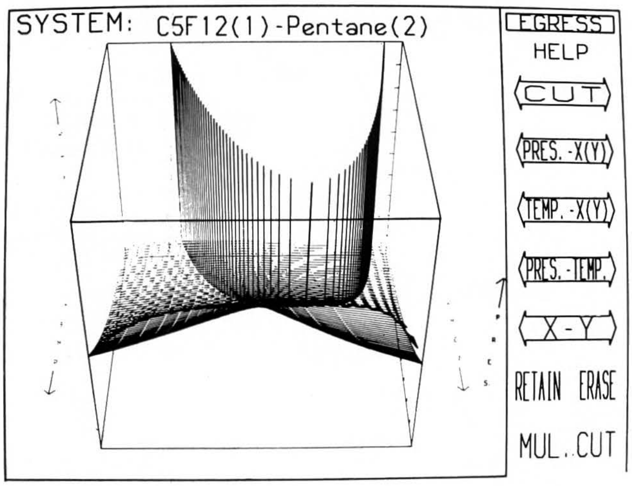

FIGURE 4. A 3-D view of another class II system, C_5F_{12} - C_5H_{12}. The original display has been rotated by 180 degrees and tilted downward so that the view is from the high-temperature end and somewhat above the phase diagram. The regions of vapor-liquid equilibria (showing an azeotrope) and liquid-liquid equilibria (solid vertical lines) are clearly visible.

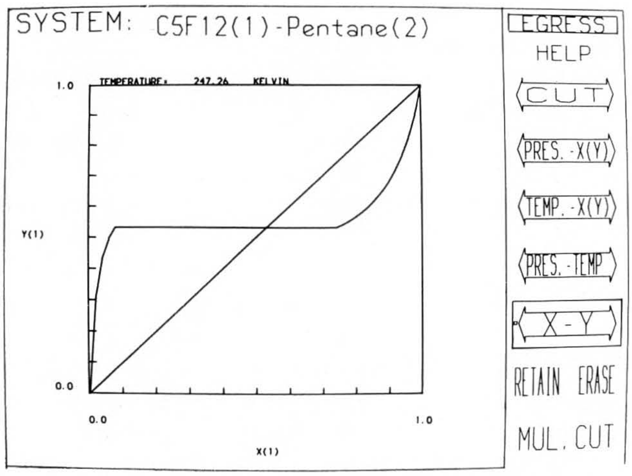

FIGURE 5. Two-Dimensional x-y diagram for the system C_5F_{12}-C_5H_{12} derived from the three-dimensional phase diagram at 247.26K. This diagram shows the characteristic behavior of an azeotropic system with liquid-liquid immiscibility, as shown by the horizontal portion of the curve.

USER INTERACTION WITH THE GRAPHICS SOFTWARE PROGRAMS

The image of the phase diagram (e.g. as in Figs. 2-6) can be manipulated by the user by means of an electronic tablet and stylus (pen). As the pen is moved over (and slightly above) the surface of the tablet, a cursor in the form of cross-hairs moves over the display. When the pen is pressed down onto the tablet the graphics program is activated and performs an operation appropriate to the area of screen chosen, given that such an area is one of the several specially designated parts of the screen called "windows" on a so-called "menu" of options.

In this application of computer graphics the menu contained the following list of 'entrées' for the user to select

a) **READ: Allows the user to choose different binary systems to examine by supplying one of a given set of data file names via the terminal.**

b) **ORBIT: This allows the phase diagram to be rotated about its pressure and composition axes in a continuous fashion as required.**

c) **PAN: Allows horizontal or vertical translation of the phase diagram.**

d) **ZOOM: Provides closer examination of a chosen area of the image by scaling the diagram up or down.**

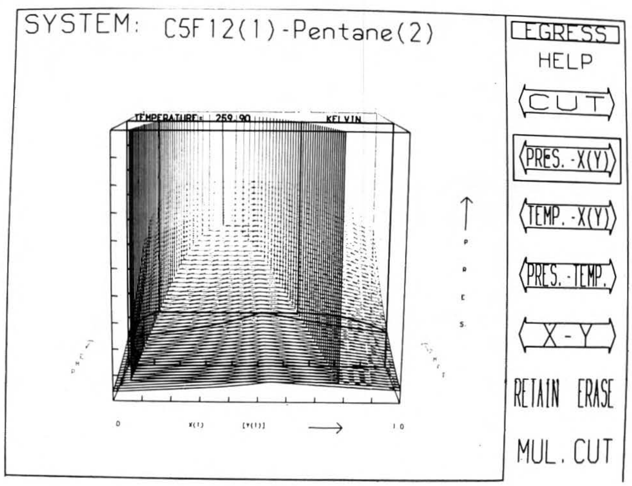

FIGURE 6. A view of the C_5F_{12}-C_5H_{12} phase diagram as it appears in the initial orientation on the screen. Solid and dashed lines have the same meaning as in Figure 2. A P-x-y cut is shown superimposed in bold on the diagram at a temperature of 259.9 K.

e) **STRETCH: Scales either of both of the P, T axes relative to the composition axis for ease of viewing.**

f) **HELP: Summons the HELP text.**

g) **RESET: Voids all previous manipulations and resets the system to the beginning of the program.**

h) **SNAP: Produces a hard-copy image of the screen on a nearby plotter.**

i) **EGRESS: Allows the user to terminate his or her session.**

j) **T-X, P-X, P-T: Each of these windows allows a particular highlighted "cut" of the phase diagram to be chosen by the user as shown in Figure 3 for a T-x cut at 0.03 bars for the system methane-carbon tetrafluoride, and in Figure 6 for a P-x cut at 259.9K for C_5F_{12}-pentane.**

k) **CUT: Produces a P-x, P-T or T-x "cut" displayed alone (i.e. not superimposed on the whole phase diagram) depending on which of these three windows (P-X, P-T or T-X) was last active. Multiple cuts (of P-x at different temperatures for example) may be displayed simultaneously.**

l) **Produces an x-y plot at constant temperature, as shown in Fig. 5 for the system C_5F_{12}-pentane at 247 K.**

A 16mm movie lasting approximately thirteen minutes has been prepared to illustrate the capabilities of this graphics package; this was presented at the 1983 AIChE annual meeting in Washington, D.C.

SUMMARY

The interactive graphics package illustrating the phase behavior of binary mixtures which has been described in this paper has been used within the chemical engineering curriculum at Cornell since the fall semester of 1982. It has proven to be extremely popular with the students, and has raised the level of comprehension of this potentially difficult subject above that achieved previously using conventional means. The major advantage lies in the suitability of computer graphics as a means of visualizing three-dimensional objects (here the PTx phase space) ; the capability of the hardware to perform rapid and continuous rotations of the image; and, perhaps most importantly, the opportunity to interact, manipulate and control the image observed on the screen, brought about by flexible "user-friendly" software. All these features combine to contribute to the success of this technique in undergraduate instruction. □

ACKNOWLEDGMENTS

It is a pleasure to thank the Gas Research Institute for partial support of this work.

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ChE book reviews

FOUNDATIONS OF BOUNDARY LAYER THEORY FOR MOMENTUM, HEAT AND MASS TRANSFER

by Joseph A. Schetz
Prentice Hall, Inc., NY (1983)

Reviewed by
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This book on Boundary Layer Theory is indicated by the author to be applicable for students in mechanical, aerospace, chemical, civil, and ocean engineering. Some people would doubt that anyone could succeed in such a broad task. The author's stated goals for this book include (i) providing an understandable coverage of advances in turbulence modeling, (ii) presenting application of large digital computers to boundary layer problems, and (iii) treating mass transfer in an integrated manner with momentum and heat transfer. It would appear that the first goal has been met reasonably well; achievement of the second goal is questionable, and the third goal has definitely not been met to the satisfaction of chemical engineers.

The book is generally well written and well-organized. The coverage of laminar flows includes chapters on integral and differential equations of flow together with approximate integral solutions and exact similarity solutions. Unfortunately almost all of this material is available in a number of other sources and hardly any of it is more recent than 1960. The meager coverage of mass