

## IMPROVEMENTS IN THE TEACHING OF STAGED OPERATIONS

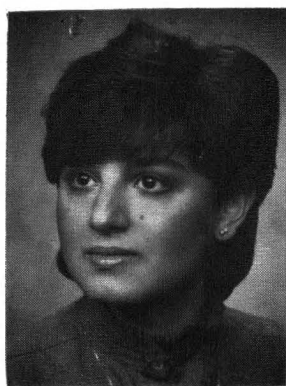
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**T**HE USE OF COMPUTER graphics to aid and improve the teaching of chemical engineering principles is an area of growing interest. Many topics have the potential to be greatly improved by utilizing the special capabilities of computer graphics, with rewards such as greater instructor efficiency and additional aid for educationally weaker students. One such topic is the teaching of staged operations, usually conducted within a separations course. For studies involving distillation—the single most important separation technique—the graphical method of McCabe and Thiele [1] is typically employed due to its conceptually simple formulation. However, the manual calculation of a single McCabe-Thiele plot for one case study is a lengthy and laborious procedure, as any junior will attest! In order to

investigate the effect of different design parameters on the resulting column, this time-consuming procedure must be repeated for each new case. The repetition involved is of limited educational value, yet it is most important that the student have a firm grasp of the interrelationship between the various operating parameters, e.g., the reflux ratio and the condition of the feed. The usual result is that a severely restricted number of cases can be studied, with additional limitations on the complexity of the system. The results of other interesting designs must be presented to the student already complete, dulling the sense of discovery that their investigation might have produced. Computer graphics offers solutions to these problems, removing the burden of computational effort while preserving the simple graphical representation which allows a ready comprehension of the situation. These advantages were recognized by Calo and Andres [2]. However, their McCabe-Thiele package was devised around the older technology of direct view storage tube graphics, which is unsuitable for interactive use.

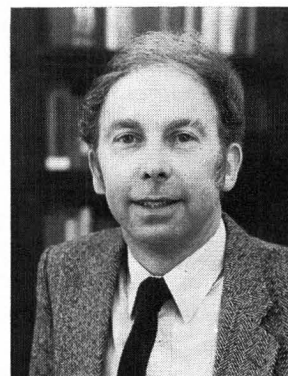
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In the graphics package developed at Cornell, the software was written for a sophisticated vector refresh graphics workstation offering superior interactive capabilities with virtually immediate response to user-interaction. This package was implemented in the fall semester of 1984, and will be used in our separations course.

### **DESIGNING THE PROJECT: HARDWARE AND SOFTWARE**

The Computer Aided Design Instructional Facility at Cornell's Engineering School has been described in an earlier publication [3]. Of the graphics workstations available, a vector refresh Evans and Sutherland Multipicture System was chosen for this application since software expertise for this type of system was available within the department. However, the nature of the application is such that it could equally well have been set up on a raster graphics system; indeed, the programs have been structured for such a change if necessary. User interaction with the package was made possible largely through the use of an electronic tablet and stylus (or pen), with a VT100 terminal for alphanumeric input. An electrostatic plotter was available for 'hard copy' output of the contents of the screen, a useful feature for the preparation of homework assignments.

As with the graphics package to represent phase diagrams developed at Cornell [3], the appearance of this software package was carefully conceived so that the design criteria given below would be fulfilled in the most effective and inviting fashion—in other words, in what computer scientists like to call a "top-down" approach. The objectives of the software package were

- For a complete set of user-supplied variables describing the system, a McCabe-Thiele plot should appear on the monitor's screen, together with a scaled diagram of the resulting distillation column.
- Interaction with the software package to change any of the design parameters should be easily effected and should produce an almost instantaneous response in recomputing the McCabe-Thiele plot and the design of the column, redisplaying them on the monitor. This interaction should be designed so that qualitative trends in column design result-

ing from parameter changes could be viewed almost continuously if desired, or that specific values for these parameters could be entered if a quantitative calculation is required.

- Extensive help must be available to aid the confused, while the ability to restore the original screen display is essential for the computationally entangled. Instructive messages should appear on the screen to inform the user of the program's status—for example, if some unavoidable delay in processing the input is about to occur.
- The program must be structured in such a way that its extension to more complex problems can be incorporated into the existing software in a straightforward manner. Thus, some long-range planning of the possible modifications to the package had to be considered.
- As far as possible the software produced should be portable, so thought had to be given to producing a machine-independent code. The decision to write the software in FORTRAN, still the most widely used high-level language in engineering, stemmed from this desire.
- Last, but still important, the programs should be "bomb-proof," even for the most inventive student user! The most likely input errors, or miskeying, must be anticipated wherever possible.

Should these objectives not be met, resulting in a final product that was difficult or frustrating to use, much of its educational impact would be lost. Such attention to detail in designing the application graphics package is extremely time-consuming in terms of software development, but the effort is amply recompensed once its use is established as a regular component of the course.

### **THE INTERACTIVE McCABE-THIELE PACKAGE**

We believe that the final product does indeed meet the criteria given above, satisfying both the instructor's and the student's differing needs. It is a routine matter to produce numerical sub-routines performing the calculations for the McCabe-Thiele plots, but more time-consuming to incorporate the graphics software to display an aesthetically pleasing picture on the screen and an ergonomically attractive interaction with the displayed image.

The layout for the display is as shown in Fig. 1. The master object displayed consists of a McCabe-Thiele plot with appropriate equilibrium and operating lines and the "ladder" of stages.

This is supplemented by a scale diagram of the corresponding design for the distillation column (relative to a six-foot tall 'stick figure' standing beside it). Above these diagrams information about the current values of the various operating parameters is displayed, while the space below is reserved for the "menu." The menu provides a selection of options to enable the user to interact with the viewed image. The user may select a particular option by moving the pen across and slightly above the tablet until the cursor (in the form of crosshairs on the screen) lies within the required area (or window) designated for this option. Pressing the tip of the pen down in contact with the tablet activates the window to perform a specific task.

The menu options for interacting with the package are listed below (the window names are in bold face type)

1. Six windows allow input of both the **composition** and the **flowrate** of the **feed**, **distillate**, and **waste** product. The program will prompt the user for values of any four independent variables from these six in order to completely define the problem. Values are entered by placing the pen down at some point within the window. Each window contains a potentiometer which allows the value of the appropriate variable to decrease or increase as the pen is moved left or right across the window. The value given by the current position of the pen may be read in the area above the diagrams.

2. When the **calculate** window is selected, the program checks to see if the mass balance was satisfied by the user-supplied variables. If the mass balance was not satisfied the user is informed and will be prompted to re-enter all four values. In this way the programs assure that the student is capable of performing the mass balance correctly. Assuming all is well, a McCabe-Thiele plot is produced for "start-up" values of the operating parameters, e.g. the reflux ratio.

3. The user may now alter these operating parameters by selecting appropriate windows for the **reflux ratio**, **operating pressure** and **heat per mole of feed**. Again, moving the pen along the length of the window alters their respective values with immediate response from the programs, producing altered images for the McCabe-Thiele plot and column design.

4. If the user desires to set an exact value for any variable this can be done using the **key in** option. This offers an alternative to using the po-

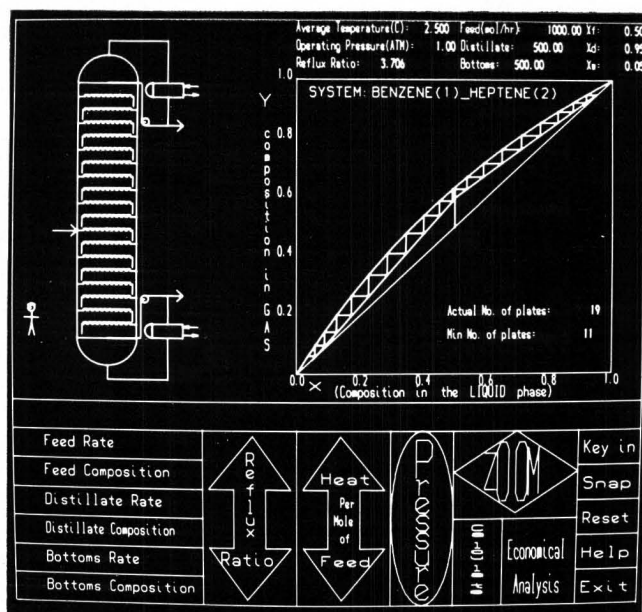


FIGURE 1

tentiometers within the windows, which are more suited to observing qualitative trends in the behavior of the McCabe-Thiele plot. The 'key in' feature prompts for numerical input at the VT100 terminal.

5. The **reset** window sets all the flowrates and compositions to zero and the operating parameters ( $p$ ,  $R$  and  $q$ ) back to their initial preset values.

6. The window marked **economical analysis** allows the user to determine the optimum value of the reflux ratio in cost effectiveness. This will be explained in more detail in the following section.

7. **Snap** triggers the production of a paper copy of the current screen contents on a nearby plotter.

8. **Help** invokes the display of information pertinent to the operation of each of the windows in turn.

9. **Exit** halts execution of the program.

## COLUMN DESIGN

The McCabe-Thiele method is widely used as an educational tool in teaching distillation column design at the undergraduate level, and details of the method need not be repeated here. In the existing version of the program, a single column involving only one feed of a binary mixture of components is considered. Extension of the programs to multiple feeds and sidestreams is underway. The feed may be introduced into the column



in any fluid condition (i.e., saturated liquid, sub-cooled liquid, etc). Antoine's equation is used to obtain the saturated temperatures and pressures of both components, and the x-y equilibrium curve is obtained assuming ideal behavior. Optional consideration of a variety of non-ideal descriptions of the equilibrium curve is also possible.

Routines are included which calculate the diameter and height of the distillation column for each case study in order to produce the scaled diagram described earlier, including the correct number of bubble-cap trays, a total condenser, reboiler, and the location of the feed tray. This is achieved by following the recipe outlined in Treybal [4].

Some interesting aspects of column design with regard to the economics involved are also incorporated by allowing the preparation of a graph showing the relationship between a given reflux ratio and the total cost involved, considering both capital costs and estimated running costs over the expected lifetime of the column. The minimum of this parabolic curve allows the estimation of an optimum reflux ratio for the most cost-effective operation of the column.

#### SUMMARY

The implementation of the computer graphics package described has proved to be of considerable assistance in the teaching of staged operations. Instructors benefit from the increased quantity and complexity of problems which can be investigated in the allotted time, and students welcome this novel and easy-to-use tool which makes completing their assignments so much less onerous. □

#### ACKNOWLEDGMENTS

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#### REFERENCES

1. McCabe and Thiele, *Ind. Eng. Chem.*, 17, 605 (1925).
2. J. M. Calo and R. P. Andres, *Comp. in Chem. Eng.*, 5, 197 (1981).
3. C. D. Naik, P. Clancy and K. E. Gubbins, *Chem. Eng. Ed.*, 19, 78, (1985).
4. R. E. Treybal, *Mass Transfer Operations*, 2nd edition (1968), McGraw-Hill, NY, p. 131-135, 142-144.

#### More on Tubular Flow Reactors

Dear Editor:

Professor Asfour's two improvements (*CEE* XIX, 2, 84, 1985) to the original design of a tubular flow reactor using crystal violet dye and sodium hydroxide reactants (Hudgins and Cayrol, *CEE* XV, 1, 26, 1981) are timely ones. This experiment, to judge from a recent survey (E. O. Eisen, "Teaching of Undergraduate Reactor Design," AIChE Meeting, San Francisco, Nov. 1984), is now incorporated into several reaction engineering laboratory courses in North America.

I welcome the occasion of the Asfour article to suggest several additional improvements that arise out of our experience since 1981.

First, I concur with the footnote in the Asfour paper. Tygon tubing is an unhappy choice for the tubular reactor. In our experience, clear Tygon tubing darkens within a few hours' use to a permanent deep violet. This obscures the pleasing axial color change that is one of the main attractions of the experiment. Polyethylene tubing, though translucent rather than transparent, resists the crystal violet dye for a much longer time.

Calculating the reactor volume can be a problem. Certainly, the nominal value of the inside diameter of the tubing is not sufficiently accurate. Some students have improved on this value by trying to fit the tubing using indexed drill bits. Because of the flexibility of the tubing, however, it is not certain that the cross-sectional area remains undistorted when the tubing is wound on the large spool. Weighing the spool with the reactor tubing empty and then filled with water appears to be the most rigorous way to obtain the volume.

In both of the above *CEE* articles, the spool is shown mounted on its side. This has proven to be an unfortunate method of mounting since bubbles often enter the reactor tubing (perhaps from the mixer pump), become trapped in the coils of the tubing, and grow. An effective remedy is to remount the spool with axis perpendicular to the lab bench and flow spiralling upward. Of course, this does not eliminate bubbles but does prevent their retention and growth sometimes to several percent of the total reactor volume.

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