Building a Computer Program: MULTICOMPONENT DISTILLATION

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In teaching stage processes to undergraduates it is usually difficult to go beyond binary systems, and analytical or graphical techniques are normally presented. Multicomponent systems requiring computer solution are more commonly encountered in industry and offer opportunities to teach undergraduates fundamentals of computer techniques at the same time they are learning the theory of stage processes. In the stage processes course given in the junior year at Cornell a multicomponent distillation program is developed in three steps (assignments) with each succeeding step incorporating the bulk of the previous program. These steps are (1) writing dew point and bubble point routines, (2) determining the approximate number of plates required in the column by a noniterative scheme based on assumed overhead and bottoms compositions, and (3) rating the column to determine the actual performance and distribution of components by an iterative technique.

The students taking the course have received an introduction to digital computers in a freshman course; consequently, the lectures on computing in this course emphasize flow charts and the assembly of large, complex computer programs from relatively simple subprograms. In developing their programs, the students are taught to regard subprograms as “black boxes” with specified inputs and outputs, as emphasized in the following quiz question:

You are given SUBROUTINE DEW which calculates the dew point temperature and the liquid composition in equilibrium with a given vapor. For a distillation column with a total condenser, specified reflux ratio, and specified distillate composition, draw a detailed flow chart to calculate the liquid composition N trays from the top.

Two weeks are allowed for each assignment to permit adequate time for debugging. After the initial writing of each program is completed, the debugging work load is sufficiently light that additional problems not requiring computer solution can be assigned in the interim.

This article describes each of the three computer programs along with the flow charts and illustrates how the computing is integrated into a course on stage processes. Flow charts and FORTRAN IV listings of each program can be obtained from the authors.

SUBROUTINES DEW AND BUBBLE

Dew point and bubble point calculations are basic to any distillation calculation and are easily coordinated with lectures on vapor-liquid equilibrium which precede the material on stage processes. For simplicity, Raoult's Law is used for calculation of K factors. In the first year the problem was used, a program for K factors was
written using the Lewis and Randall Rule and data from the generalized fugacity charts. Although the program worked well, the additional complexity of this program confused most students; thus in later years only Raoult’s Law was used.

\[ K_i = \frac{y_i}{x_i} = \frac{P_i^*}{\pi} \]

where \( y_i \) is vapor mole fraction of component i; \( x_i \) is liquid mole fraction of component i; \( \pi \) is total pressure; and \( P_i^* \) = vapor pressure of component i.

Vapor pressures were determined by the two-constant Antoine equation.

\[ \ln P_i^* = A_i + \frac{B_i}{T} \]

where \( A_i, B_i \) are Antoine constants and T is temperature, °K.

Students read in two vapor pressures with corresponding temperatures for each component. The Antoine constants are calculated once, and then used for all vapor pressure calculations. Calculation of vapor pressures was a useful problem assigned at the start of the course to enable students to review basic input/output operations.

The Newton-Raphson method is used in both subroutines DEW and BUBBLE. This method was not entirely new to most students, but the techniques used in generating the computer proved to be different and interesting. After converging to within a specified tolerance (\( \epsilon \)) the compositions are normalized. The flow chart for BUBBLE is quite similar to that for DEW (Fig. 1).

**THE DESIGN CASE**

The approximate number of plates in the column and the feed plate location can be determined by sequential material balance and equilibrium calculations repeated throughout the length of the column. DEW is used for equilibrium calculations when calculating down from the top and BUBBLE when calculating up from the bottom. Constat molal overflow is assumed. For this problem, the composition of a four-component liquid feed at its boiling point is specified along with specifications for the light key (component 2) in the bottoms and heavy key (component 3) in the distillate. For this calculation the mole fraction of the lighter-than-light key (component 1) is set to zero in the bottoms, and the mole fraction of the heavier-than-heavy key is set to zero in the distillate, permitting very close hand calculation of distillate and bottoms flow rates and composition as input to the computer.
rectifying section of the column. Similarly the number of plates in the stripping section, NBELOW, is found by stepping up from the reboiler plate by plate until the ratio of the light and heavy keys is greater than in the feed stream. (Fig. 2).

This problem is shown to be merely an extension of the McCabe-Thiele method to multicomponent systems. The flow chart analysis and computer algorithm enable the student to visualize each step in the McCabe-Thiele method, thus helping to overcome the usual tendency for a student to visualize the McCabe-Thiele method without knowing what each step represents. Very little lecture time is required to go from binary distillation to the multicomponent case. Quiz questions relate the flow chart for this problem to other stage processes, e.g., given a subroutine to calculate the equilibrium composition in a liquid-liquid extraction process with counter-current mixer-settlers, draw a detailed flow chart for calculating down N stages.

THE RATING CASE

Once the number of trays and the feed plate location are known, the exact distillate and bottoms compositions are determined using the Thiele-Geddes method as detailed by Peiser. Occasionally it is necessary to add or subtract a plate to the rectifying or stripping section to achieve the required separation.

Estimates of the distillate and bottoms compositions are used for an initial calculation through the column. In contrast to the design problem, non-zero values must be used as initial estimates for all components, and very small mole fractions on the order of $10^{-7}$ are normally given as initial estimates of the mole fraction of the lighter-than-light key in the bottoms and for the heavier-than-heavy key in the distillate. Calculating down to the feed plate and up to the feed plate shows that the component molal input AIN, and output AOUT, to the rectifying section (“A”) are not equal. The same is true of the input BIN, and the output BOUT, to the stripping section (“B”). The Thiele-Geddes procedure applies this mismatch at the feed plate to correct the initial estimates of the distillate and bottoms compositions. A simple algorithm to reduce this mismatch is

$$\frac{XD_1}{XB_1} \left|_{\text{new}} = \theta_1 \frac{XD_1}{XB_1} \right|_{\text{old}}$$

$$\theta_1 = \left[ \frac{AIN}{AOUT} \right] \frac{BOUT}{BIN} \right]^{1/2}$$

It will be noted that $\theta_1$ is greater than unity, the next estimate of XD, will be increased and the next estimate of XB will be decreased. The square root is used to evaluate $\theta_1$ rather than a linear relationship in order to reduce instability. Combining this new ratio of XD/XB, with a mass balance gives the new distillate and bottoms compositions for the next iteration. Unfortunately these mole fractions do not necessarily sum to one and a factor “C” is calculated to correct $\theta_1$ so that the distillate and bottoms mole fractions sum to one.

$$\frac{XD_2}{XB_1} \left|_{\text{new}} = C\theta_1 \frac{XD_2}{XB_2} \right|_{\text{old}}$$

“C” is calculated by a Newton-Raphson iteration using an initial estimate of $C = 1$.

At this point in the flow chart (Fig. 3) the new values of the distillate and bottoms composition are known and it is necessary to decide whether
another iteration is necessary. Since each \( \theta \) approaches unity, \( \text{ABSUMT} \) converges arbitrarily close to zero and a tolerance of 0.01-0.03 is usually sufficient.

\[
\text{ABSUMT} = \sum_{i=1}^{n} \left| \frac{1}{\theta_i} - 1 \right|
\]  

(6)

Even with the simplifying assumptions of Raoult’s Law, ideal stages, and constant molar overflow, the student feels a sense of achievement in designing and rating a multicomponent distillation column. For most students this is the first time they have generated a computer program of such complexity. Students see each step as a typical assignment and do not sense the magnitude of the project until one of them procrastinates and attempts to complete the third step without completely debugging the first two. For the normal student, debugging step three (the rating case) without incorporating the debugged form of step two (the design case) was disastrous. Most students solved the problems sequentially and truly enjoyed solving a ‘real problem’. During the several years in which they have been used, these problems generated enthusiasm which has carried over into the other elements of the course.

**STUDENT RESPONSE**

Learning to use flow charts while developing the computer algorithms enable students to use with confidence existing library subprograms. For example, after a preliminary hand calculation of a gas absorber design, students are asked to find the optimal operating conditions by using the program developed and kindly supplied by Brockmeier and Himmelblau. Because students had earlier experience in building a complex multicomponent distillation routine from subroutines, they had little difficulty incorporating the Brockmeier and Himmelblau subprogram into a calling routine of their own writing. Overall, incorporating computer methods into the undergraduate chemical engineering program by intergrating this subject into the staged operations course was clearly beneficial and well received by the students.

**REFERENCES**


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**PROGRAM COMMITTEE**

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Over the past few years it has become more and more evident that the technical programing of our AIChE meetings has become more diverse. This is because the role of the chemical engineer has been broadened to include contributions to environmental, health, and food and energy production problems of society at large. This broadening of horizons is essential for maintaining the vitality of our professional society and will be encouraged wherever possible. However, there seems to have developed over the years a noticeable division between academia and industry and in the dissemination of research results and in the dialogue which should have followed these disclosures. The tendency in the past few years is to have sessions developed by academic personnel reporting on specific academic research, and presented essentially to other academic research personnel. The situation has evolved with sessions developed by industrial personnel. Such a situation is certainly not in the best interests of either group, particularly when one group is trying to prepare young people to step into roles of responsibility in the other group.

There are certainly many factors which have led to this gradual decrease in dialogue between academia and industry. Many of these are entirely beyond the control of AIChE and the National Program Committee. Nevertheless, the Executive Board of the National Program Com-