DISTILLATION CALCULATIONS WITH A PROGRAMMABLE CALCULATOR

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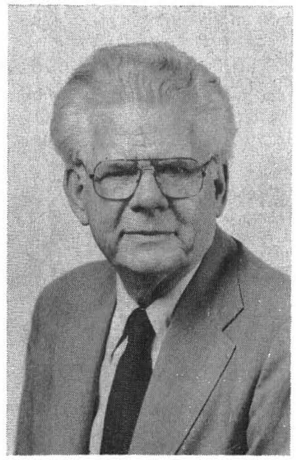

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THE CONCEPTS OF MINIMUM reflux ratio and optimum feed tray location in distillation problems involving more than two components are somewhat more difficult for students to grasp than are these concepts applied to two-component systems. These concepts can be developed from fundamentals by considering zones of constant composition and ratios of key components, using either analytical solutions (such as the Underwood equations) or stage-to-stage calculations. They can also be developed with the use of computers by calculating and plotting results for the distillation of a particular multicomponent system for a specified separation of various reflux ratios and various feed tray locations. The concept of minimum reflux ratio becomes very real when mole fractions <0 or >1 appear in printouts.

One reasonable way to approach the teaching of multicomponent distillation to undergraduates is in three steps:

1. **Develop equilibrium relations and operating line equations for the simplest case of constant relative volatility and constant molal flow rates of liquid and vapor streams.**
2. **Assign students to study patterns of distribution by performing stage-to-stage calculations for a specified separation of a four-component mixture at several reflux ratios (including at least one below the minimum) and several feed tray locations.**
3. **Generalize the results of student calculations and develop criteria for minimum reflux ratio and optimum feed tray location.**

The emphasis here on a study of patterns of distribution as an aid to understanding separation processes is in accord with C. J. King's approach as outlined in his book on separation processes.

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Step 2 of this approach can also be carried out handily with programmable calculators, providing students with the convenience of studying anywhere they please rather than having to seek out a computer terminal. The time required with a programmable calculator is quite reasonable. With the programs developed here it is possible to perform calculations for several cases in the course of one evening.

Consider the distillation of a six-component mixture.* Assume constant relative volatility and constant molal overflow. The basic equations can be written as follows:

*The TI-58C provides enough memories and program steps for more than six components.

$$y_i = \alpha_i x_i \Big/ \sum_{i=1}^{6} \alpha_i x_i$$

$$x_{i,m+1} = \frac{\bar{L} - b}{\bar{L}} y_{i,m} + \frac{b}{\bar{L}} y_{i,b}$$

$$x_{i,n+1} = \frac{L + d}{L} y_{i,n} - \frac{d}{L} x_{i,d}$$

Here the operating lines have been written in the form convenient for calculations up a column, beginning at the stillpot. These equations contain 20 constants for the six-component case for a given feed composition, feed condition, desired separation, and reflux ratio.

Register assignments and programs for stage-to-stage calculations on the distillation of a six-component mixture are presented in Table 1. Note that registers 01-06 are reserved for storing successive values of x_i and y_i. These values can be recalled as needed for recording or plotting. Programs in Table 1 are also suitable for calculations on 2-, 3-, 4-, or 5- component mixtures provided zeroes are stored in registers designated for the missing components.

The use of these programs for a case where the bottoms product composition is known is straightforward. After placing values of $x_{i,b}$ in registers 01-06, depressing key A will result in calculation of the composition of vapor leaving the stillpot. Depressing key D then yields the composition of liquid leaving the first tray above the stillpot. Alternating between keys A and D is thus all that is needed to calculate up the column. Calculations above the feed tray consist of depressing keys A and A′ alternately.

As an example of the use of these programs consider a simple case of distillation of a four-component mixture.

Component	mole % in feed	Relative volatility
1	40	2.7
2	20	1
3	15	0.76
4	25	0.35

TABLE 1
Six-Component Distillation Calculations
TI-58C Programmable Calculator
(Partition to 239/29)

ASSIGNMENTS OF REGISTERS		EQUILIBRIUM CALCULATION	OPERATING LINES: Stripping	OPERATING LINES: Rectifying
01	$x_1(y_1)$	2nd Lbl A	2nd Lbl D	2nd Lbl A′
02	$x_2(y_2)$	0	6	6
03	$x_3(y_3)$	STO 13	STO 00	STO 00
04	$x_4(y_4)$	6	20	27
05	$x_5(y_5)$	STO 00	STO 13	STO 13
06	$x_6(y_6)$	12	2nd Lbl E	2nd Lbl B′
07	α_1	STO 28	RCL 14	RCL 21
08	α_2	2nd Lbl B	2nd Prd 2nd Ind 00	2nd Prd 2nd Ind 00
09	α_3	RCL 2nd Ind 28	RCL 2nd Ind 13	RCL 2nd Ind 13
10	α_4	2nd Prd 2nd Ind 00	SUM 2nd Ind 00	INV SUM 2nd Ind 0
11	α_5	RCL 2nd Ind 00	1	1
12	α_6	SUM 13	INV SUM 13	INV SUM 13
14	$(\bar{L} - b)/\bar{L}$	1	2nd Dsz 0	2nd Dsz 0
15	$(b/\bar{L})x_{1,b}$	INV SUM 28	E	B′
16	$(b/\bar{L})x_{2,b}$	2nd Dsz 0	R/S	R/S
17	$(b/\bar{L})x_{3,b}$	B		
18	$(b/\bar{L})x_{4,b}$	6		
19	$(b/\bar{L})x_{5,b}$	STO 00		
20	$(b/\bar{L})x_{6,b}$	2nd Lbl C		
21	$(L + d)/L$	RCL 13		
22	$(d/L)x_{1,d}$	1/x		
23	$(d/L)x_{2,d}$	2nd Prd 2nd Ind 00		
24	$(d/L)x_{3,d}$	2nd Dsz 0		
25	$(d/L)x_{4,d}$	C		
26	$(d/L)x_{5,d}$	R/S		
27	$(d/L)x_{6,d}$			

The overhead product is to contain 99 mole % A, and the recovery of A is to be 99%. With these specifications it is reasonable to assume that the overhead contains only A and B, and a good estimate of the bottoms composition can be made:

$$x_{1,b} = 0.0067$$
$$x_{2,b} = 0.3267$$
$$x_{3,b} = 0.2500$$
$$x_{4,b} = 0.4166$$

A first assignment for calculations in this case could be as follows:

1. **For a reflux ratio in the range L/d = 1 – 2, calculate up the column until a zone of constant composition is reached. Prepare a plot of liquid composition vs. plate number. Select a reasonable tray for introducing the feed and calculate up the column to the product composition. Try two more feed tray locations. Which choice of feed tray requires the minimum number of trays for the specified separation?**
2. **Study the effect of decreasing L/d. Try a series of values until you reach a value where the specified separation can not be achieved. What happens?**
3. **Rewrite the problem for a case where a split is to be made between components 2 and 3. For example, specify that recovery of B in the overhead is to be 99% and recovery of C in the bottoms is to be 99%.**

With these exercises behind them, students are well prepared for more formal developments of multicomponent distillation calculations.

The results of calculations for a reflux ratio (L/d) of 1.2 are summarized in the Table below and in Fig. 1. Tray 8 was selected as the feed tray after inspecting a graph of tray number vs. mole fraction in which calculations were performed from still to a pinch region (at about tray 18).

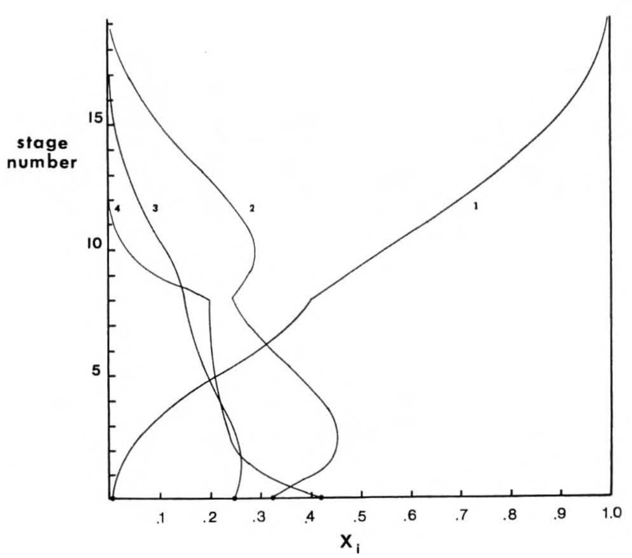

FIGURE 1. Results for L/d = 1.2

Summary of Results for L/d = 1.2

Tray number	x_1	x_2	x_3	x_4
Still	0.0067	0.3267	0.2500	0.4166
2	0.0410	0.4531	0.2574	0.2485
4	0.1417	0.4205	0.2174	0.2204
6	0.3001	0.3181	0.1756	0.2061
8	0.4058	0.2449	0.1516	0.1978
10	0.5676	0.2916	0.1103	0.0305
12	0.7105	0.2321	0.0542	0.0032
14	0.8402	0.1388	0.0207	0.0003
16	0.9311	0.0623	0.0066	1.7431×10^{-5}
18	0.9814	0.0167	0.0019	1.0564×10^{-6}
(y_{18})	(0.9932)	(0.0063)	(0.0005)	(1.3858×10^{-7})

Values of x and y can be recorded for each tray, of course, but liquid mole fractions on even-numbered trays were chosen here as sufficient to define a graph of tray numbers vs. liquid mole fraction. □

Editorial Note: A more complete set of programs providing for calculations beginning at either the top or bottom of a column is available and can be obtained by contacting either of the authors of this article.

NOMENCLATURE

x_i = mole fraction of ith component in liquid.
y_i = mole fraction of ith component in vapor.
α_i = relative volatility of ith component.
L = Liquid flow rate in rectifying section, moles/hr.
$\overline{L}$ = Liquid flow rate in stripping section, moles/hr.
b = Flow rate of bottoms product, moles/hr.
d = Flow rate of overhead product, moles/hr.
m + 1 refers to plate above mth plate in stripping section.
n + 1 refers to plate above nth plate in rectifying section.

BOOK REVIEW: Alternative Fuels

Continued from page 85.

plications of these fuels, and with the unconventional fuels that can be derived from both conventional and unconventional fuels. The author then examines and compares each of the alternatives in terms of combustion characteristics, and combustion performance.

The last chapter is devoted to those fuels which appear to hold particular promise, which are coal conversion products, alcohol and hydrogen.

This book is informative and may be useful as a reference in an introductory course on fuel. □