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Nomenclature

C = concentration
 t = contact time
 E_a^0 = equilibrium distribution coefficient
 T = temperature
 A = extracted species
 B = stored species
 R_1 = uranium extraction rate constant

Subscripts

i = initial
 f = final
 t = at a given time

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Approximate Solutions for Distillation Rating and Operating Problems Using the Smoker Equations

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Algorithms for rapid solution of implicit variables in the Smoker design equations are presented. The accuracy of these solutions in the context of distillation rating and operating problems is evaluated for distillation systems where more rigorous physical property assumptions are known to apply. Alternative methods of initially fitting the Smoker equations to rigorous tray-by-tray material and energy balance calculations as well as methods extending the procedure to handle multicomponent systems are discussed. These methods are well suited for many optimization, reliability, and control studies as well as for the fast real-time calculations such as interactive computations or on-line control.

Introduction

Recently there has been a great deal of interest in short-cut or approximate solution techniques for distillation calculations. These short-cut methods are useful for preliminary evaluation studies, optimization problems, design reliability calculations, process control studies, real-time control algorithms, interactive computations (CAD), and programmable calculator programs.

One such method receiving interest anew is the analytical solution to the McCabe-Thiele diagram first presented by Smoker (1938). A paper by Strangio and Treybal (1974) discussed the advantages of using an analytical approach over the various popular empirical methods most of which are based upon correlations of Gilliland's (1940) data. Their paper presented a design algorithm which simultaneously satisfied the minimum number of stages, $N_m = f(x_b, x_d, \alpha)$ (Fenske, 1932); the minimum reflux ratio, $R_m = f(q, x_d, x_f, \alpha)$ (Underwood, 1948); and the number of stages at a specified reflux ratio, $N = f(q, x_f, x_d, x_b, R, \alpha)$ (Smoker, 1938).

In addition to the design problem, a series of papers by McAvoy (1977), Jafary et al. (1979a), and Douglas et al. (1979) discuss the use of the Smoker equations for control and operability studies. As they point out, these equations are explicit in the design variables (N_r and N_s), but must be solved iteratively for the operating or controlled variables (D, B, L_r, V_s, x_b , or x_d). They proceed to present various alternate approximating equations that are valid under certain regions of column operation. These approximations are shown to be somewhat better than the empirical estimation procedures used by Shinskey (1977) for column control analysis. However, even these approximate solutions have been found unsatisfactory for columns operating close to their minimum reflux ratio and also for high-purity columns where the product impurities at one or both ends of the column are less than 1%.

Efficient iterative algorithms for rapid solution of these implicit operating variables will now be presented. The use of iterative calculations is entirely satisfactory as long as convergence is guaranteed and rapidly achieved. These new algorithms have been applied to binary columns where the product compositions ranged from equal to the feed, down to impurity levels as low as one part per million. Computational accuracy of one part per million requires between 5 and 10 iterations, and intermediate calculations

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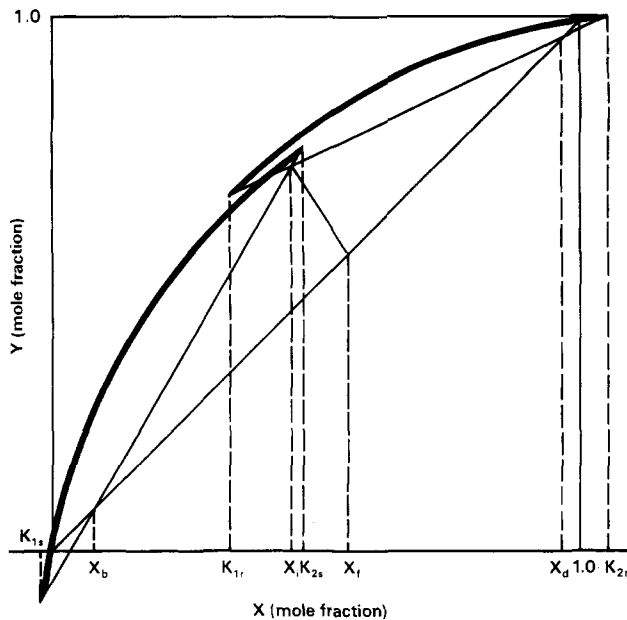


Figure 1. The Smoker equation variables illustrated on a McCabe-Thiele diagram.

must be accurate to 12 significant figures. Both these speed and accuracy requirements can be achieved in most present hand-calculators and minicomputers.

Algorithm Development

Two algorithms have been developed, one for rating problems and one for operating problems. The first type of calculation is the rating problem in which the column, the feed, and the operating variables are specified and the product compositions are to be determined. Variations of this problem include specification of one product composition and one operating condition. The other type of calculation is the operating problem in which the column, the feed, and both product compositions are specified and the required distillate and reflux flows are to be determined. This latter calculation is subject to the restriction that the given column can in fact achieve the specified product compositions for the feed conditions indicated.

The two algorithms are developed starting with the Smoker design equations for the rectifying and stripping sections of a binary distillation column under the assumptions of constant relative volatility and equal molal overflow. The equations are derived by recognizing that for each section, the equilibrium curve and operating line intersect at two locations. These curves are illustrated in Figure 1 for a column with constant, but different, relative volatilities in its rectifying and stripping sections.

The points of intersection for these curves may be determined by solving the two equations for each section simultaneously. The equation for an equilibrium curve with constant relative volatility is

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} \quad (1)$$

and the equation for a constant L/V operating line resulting from the equal molal overflow assumption is

$$y = mx + b \quad (2)$$

The two roots may then be calculated as

$$K_1 = \frac{-(m + b(\alpha - 1) - \alpha) - [(m + b(\alpha - 1) - \alpha)^2 - 4mb(\alpha - 1)]^{1/2}}{2m(\alpha - 1)} \quad (3)$$

$$K_2 = \frac{b}{m(\alpha - 1)K_1} \quad (4)$$

The first of these roots is always the smaller of the two, as is indicated in Figure 1.

After shifting the coordinate axis, Smoker was able to derive a recursive equation for the X coordinate of the N th stage along the operating line. If both the starting and final compositions of a section were specified, the equation could be solved for the number of stages, N .

Following the approach taken by Jafary et al. (1979b), the Smoker equations for each section of the column may be written as a function of the product compositions, the two roots, and an intermediate composition common to each equation

$$N_r = \left\{ \ln \left[\frac{(x_d - K_{1r})(K_{2r} - x_1)}{(x_1 - K_{1r})(K_{2r} - x_d)} \right] \right\} / \left\{ \ln \left[\frac{1 + (\alpha_r - 1)K_{2r}}{1 + (\alpha_r - 1)K_{1r}} \right] \right\} \quad (5)$$

$$N_s = \left\{ \ln \left[\frac{(x_i - K_{1s})(K_{2s} - x_b)}{(x_b - K_{1s})(K_{2s} - x_i)} \right] \right\} / \left\{ \ln \left[\frac{1 + (\alpha_s - 1)K_{2s}}{1 + (\alpha_s - 1)K_{1s}} \right] \right\} \quad (6)$$

where K_{1r} and K_{2r} are the roots for the rectifying section, K_{1s} and K_{2s} are the roots for the stripping section, and x_i is the intermediate composition determined by the intersection of the two operating lines (and also the "q-line", representing feed enthalpy), as shown in Figure 1. At this point, McAvo (1977) suggests combining eq 5 and 6 in order to eliminate the intermediate composition, x_i . This elimination is carried out by first solving both equations for x_i and then setting the two right-hand sides equal to each other. The task is made easier by first defining the terms C_r and C_s as

$$C_r = \left[\frac{1 + (\alpha_r - 1)K_{2r}}{1 + (\alpha_r - 1)K_{1r}} \right]^{N_r} \quad (7)$$

$$C_s = \left[\frac{1 + (\alpha_s - 1)K_{2s}}{1 + (\alpha_s - 1)K_{1s}} \right]^{N_s} \quad (8)$$

The intermediate compositions may now be expressed as

$$x_{ir} = \frac{C_r K_{1r}(K_{2r} - x_d) + K_{2r}(x_d - K_{1r})}{C_r(K_{2r} - x_d) + x_d - K_{1r}} \quad (9)$$

$$x_{is} = \frac{C_s K_{2s}(x_b - K_{1s}) + K_{1s}(K_{2s} - x_b)}{C_s(x_b - K_{1s}) + K_{2s} - x_b} \quad (10)$$

where x_{ir} is the intermediate composition determined from the rectifying equation, and x_{is} is the same composition determined from the stripping equation.

The resulting equation when eq 9 and 10 are set equal may be thought of as a separation relationship which must be satisfied simultaneously along with the material balance equation for the column. In order to solve these simultaneous equations, McAvo first solved eq 9 for x_d in terms of x_{is}

$$x_d = \frac{C_r K_{1r}(x_{is} - K_{1r}) + K_{1r}(K_{2r} - x_{is})}{C_r(x_{is} - K_{1r}) + K_{2r} - x_{is}} \quad (11)$$

and then proposed the following iteration procedure. For the rating type problem, assume x_d , use the material balance equation to determine the second unknown, calculate x_{is} from eq 10, and then calculate x_d from eq 11 as a check on the assumed value. The equation

$$f(x_d) = x_d(\text{calcd}) - x_d(\text{assumed}) = 0 \quad (E1)$$

may be solved by a root-finding technique to give the correct solution to the rating type problem.

Similarly, if x_b is to be assumed initially, eq 10 may be solved for x_b in terms of x_{ir}

$$x_b = \frac{C_s K_{1s} (K_{2s} - x_{ir}) + K_{2s} (x_{ir} - K_{1s})}{C_s (K_{2s} - x_{ir}) + x_{ir} - K_{1s}} \quad (12)$$

then in a like manner the equation

$$f(x_b) = x_b(\text{calcd}) - x_b(\text{assumed}) = 0 \quad (E2)$$

may be solved.

For the operating type problem in which the distillate and reflux flows are to be determined, D can be calculated from the material balance equation and then either of the following equations may be solved

$$f(R) = x_d(\text{calcd}) - x_d(\text{given}) = 0 \quad (E3)$$

or

$$f(R) = x_b(\text{calcd}) - x_b(\text{given}) = 0 \quad (E4)$$

Unfortunately, the functions in eq E1–E4 are of a form ill-suited for iterative computations. An indication of this difficulty is the 0.1 damping factor required in the direct iteration scheme proposed by McAvoy. Solutions to one part per million accuracy require hundreds of functional evaluations even for relatively easy separations.

Examination of these functions for several hundred distillation problems has led to the following observations. For columns operating with their D/F ratio approximately equal to x_f , the light key composition in the feed, all four of these functions will have both a root and a pole in the feasible solution region and will typically behave as shown in Figure 2. For the functions in eq E1 and E2 the pole always occurs at a higher purity than the root and for the functions in eq E3 and E4 the pole always occurs at a lower reflux ratio than the root.

For problems in which the D/F ratio is much larger than x_f , the pole for the functions in eq E2 and E4 moves outside the feasible solution region making those functions much easier to solve. Likewise, in problems with the D/F ratio much less than x_f , the pole for the functions in eq E1 and E3 moves outside the feasible solution region. In most practical problems, however, both the root and pole exist in the region to be searched, and all of the more rapid iterative solution techniques fail to converge under these circumstances. Methods which first bracket a root are still inefficient because the root and pole are relatively close, differing by less than 1% of the search interval, and a very small step size is thus required to insure success.

In order to avoid this dilemma, the following alternative approach is proposed. Instead of eliminating the intermediate composition, its value is computed from both the rectifying and the stripping sections using eq 9 and 10. Then, depending upon the problem at hand, one of the following new equations may be solved

$$f(x_d) = x_{ir} - x_{is} = 0 \quad (E5)$$

or

$$f(x_b) = x_{ir} - x_{is} = 0 \quad (E6)$$

or

$$f(R) = x_{ir} - x_{is} = 0 \quad (E7)$$

The new functions in eq E5–E7, though similar to those proposed by McAvoy, exhibit much better behavior and are well suited for iterative root-finding techniques. For example, in all problems, the function in eq E5 increases monotonically and has only a single root in the search interval. Likewise, the functions in eq E6 and E7 decrease

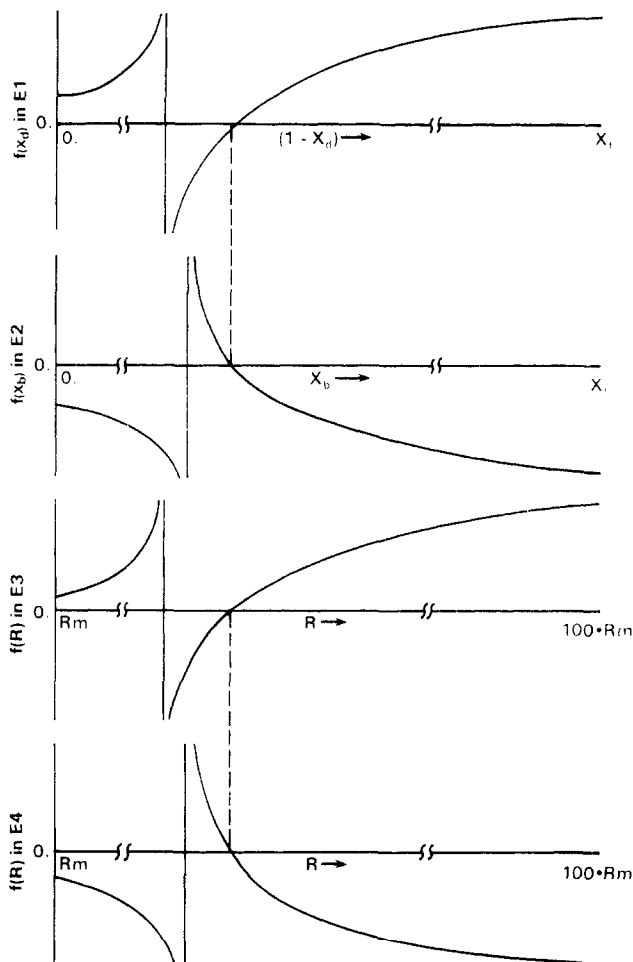


Figure 2. Functions which result from elimination of the intermediate composition.

monotonically and also have only one root. If a simple iterative solution technique such as rational fraction interpolation (Chien, 1972) is applied, the correct solution may always be obtained in 5 to 10 iterations to a computational accuracy of one part per million.

Evaluation

Since rapid solution of the analytical equations is now possible, it is worthwhile to consider the validity of these solutions in the context of the rating type problem. The source of error introduced in using these equations to approximate a distillation column are: (1) the vapor–liquid equilibrium relationship and tray efficiencies which differ from the constant relative volatility assumption, and (2) the vapor and liquid molal enthalpies which differ from the equal molal overflow assumption.

The net effect of these errors may be ascertained by comparing results obtained from use of these equations to solutions obtained from tray-by-tray material and energy balance calculations made with more rigorous physical property models. First, a rigorous design or base case is determined and the Smoker equations are “fitted” to the results. Next, the Smoker rating algorithm is applied to obtain approximate solutions for parametric cases about the base case. Solutions to these same parametric cases are computed with tray-by-tray balances using the more rigorous physical properties and they serve as a check on the approximate solutions.

In order to fit the Smoker algorithms to the rigorous base case solution, the relative volatility is first determined on each tray and then a geometric average is computed for the stripping and rectifying sections of the column. This method appears to give acceptable results in most cases,

even for rather nonideal solutions.

Nonlinear operating lines present somewhat more of a problem, perhaps because their effect is less well understood (Chien, 1978). At first, an approach similar to that suggested by Douglas et al. (1979) was evaluated. In this approach, which will be referred to as the N -fit method, the actual external reflux and boilup ratios are used to compute an equivalent number of stages for each section of the column. The equivalent number of stages takes into account not only the nonlinear operating lines but also tray efficiencies for each section of the column. This approach results in a model with a pseudo feed quality and would not be feasible when straight operating lines do not project to an intersection under the equilibrium curves. The use of the Smoker design equations also forces an optimal feed tray location since x_i is specified as the intersection of the operating lines. For any column with a poorly matched feed tray, the equivalent number of stages computed in each section will be seriously in error.

Several alternative approaches to fitting the operating lines have been evaluated. As a result of these studies, the following L -fit method is recommended because it will always yield a feasible model and is generally more accurate than the other methods examined. First, actual vapor compositions determined from Murphree vapor efficiencies are used to compute pseudo-relative volatilities on each tray, and these are geometrically averaged as before. The operating algorithm (E7) is then used to determine a reflux ratio necessary to achieve the product specifications for the given column and feed under linear operating line and constant relative volatility assumptions. This algorithm uses the actual number of trays in each section of the column and x_i , the intermediate composition, is not restricted to occur at the intersection of the operating lines. A much better fit for columns with poorly located feed trays can thus be made.

A pseudo-internal reflux ratio is then defined as the Smoker reflux divided by the actual external reflux

$$G = \frac{L_{R(\text{Smoker})}}{L_{R(\text{actual})}} \quad (13)$$

In order to determine the reflux to be used in the rating algorithms (E5 or E6), changes to the actual external reflux are first multiplied by this ratio. This approach has the advantage of being inherently able to handle columns with a subcooled external reflux; however, the simple ratio of these refluxes as opposed to a slope-intercept relationship introduces an additional source of error.

Results

Three distillation systems have been chosen to illustrate typical results obtained: acetone-benzene, benzene-toluene, and benzene-monochlorobenzene (MCB). The rigorous tray-by-tray calculations are performed by the FRAKB distillation block in the FLOWTRAN (Trademark, Monsanto Co. The FLOWTRAN computer program is licensed by Monsanto.) material and energy balance program. Physical property data and correlations used for the FLOWTRAN simulations are discussed in the Appendix. These three systems were chosen for their progressively less ideal equilibrium data. Furthermore, three different separation tasks were selected. These included a non-symmetric separation with a high purity overhead product (<0.1%), a more-or-less symmetrical separation with two high-purity products (both <0.1%) and another nonsymmetric separation with a very high purity bottom product (<100 ppm).

The columns were then each specified to operate at approximately 1.2 times the minimum reflux ratio which

Table I. Base Case Design and Smoker Fit Data

design data	example 1	example 2	example 3
F	100.0	100.0	100.0
D	49.49	65.03	35.53
$x_f \times 100$	45.0	65.0	35.0
$x_b \times 100$	0.9837	0.0272	0.0041
$(1 - x_d) \times 100$	0.0811	0.0607	1.4991
q	1.101	1.211	1.161
q (N -fit)	1.057	1.107	1.115
N_r	18	19	8
N_r (N -fit)	18.55	17.99	5.70
N_s	14	17	16
N_s (N -fit)	12.29	17.97	16.76
L_r	107.2	85.58	32.19
L_r (L -fit)	104.9	82.45	26.67

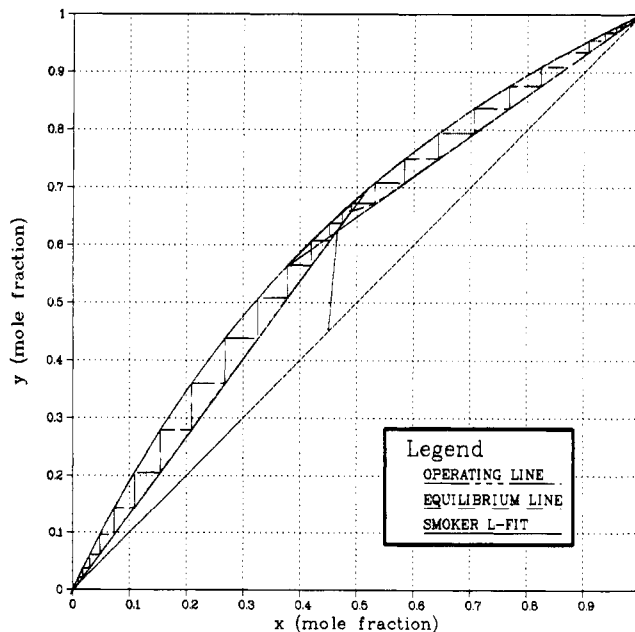


Figure 3. The Smoker L -fit for example column 1, acetone-benzene.

is generally considered to be an optimal economic design. Subcooled feeds were specified, and saturated external reflux flows were used in order to directly specify the operating parameters for these parametric cases. For each of these examples the distillate product was specified as a liquid; however, a vapor distillate product may be specified instead.

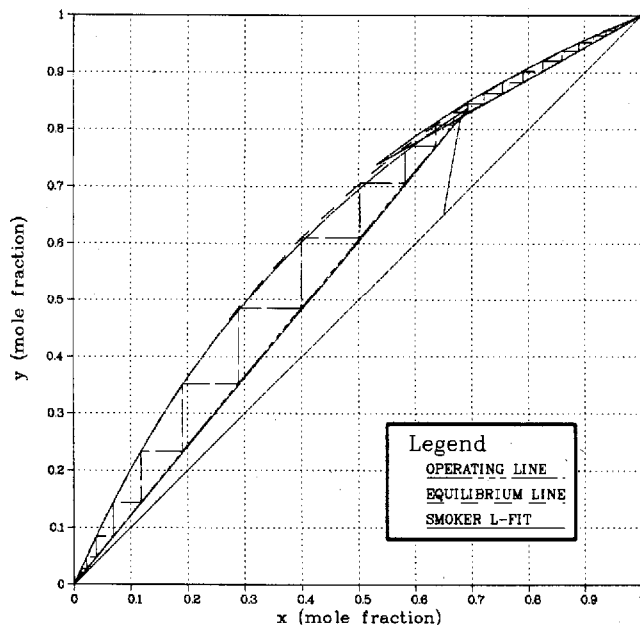
For each example column, the base case design data and the fit of the Smoker equations as determined by the N -fit and L -fit methods are shown in Table I. For the distillate composition, product impurity is given so that the results may be compared on the same basis as the bottom product. The compositions have been multiplied by 100 to convert the mole fractions to mole percent.

Example column 1, the acetone-benzene separation, is shown in Figure 3. The McCabe-Thiele diagram is generated from the FLOWTRAN output and is not at constant pressure but rather includes a realistic pressure drop across each tray. The Smoker L -fit to the column has then been superimposed to illustrate the validity of the constant relative volatility and straight operating line assumptions. The same information for example columns 2 and 3, the benzene-toluene and benzene-MCB separations respectively, is shown in Figures 4 and 5.

The results of six parametric cases about the base case for each column are presented in Table II. These six cases include positive and negative deviations, both 1 and 10% changes to the material balance (D/F) with constant reflux

Table II. Parametric Cases Comparing FLOWTRAN FRAKB Solutions to Corresponding Smoker Solutions

parametric case	sol'n method	example 1		example 2		example 3	
		$x_b \times 100$	$(1-x_d) \times 100$	$x_b \times 100$	$(1-x_d) \times 100$	$x_b \times 100$	$(1-x_d) \times 100$
base case	all	0.9837	0.0811	0.0272	0.0607	0.0041	1.4991
+1.0% D/F	N-fit	0.3998	0.3449	0.0020	0.9910	0.0005	2.4807
	FRAKB	0.2966	0.2186	0.0065	0.9935	0.0022	2.4836
	L-fit	0.2811	0.1995	0.0035	0.9918	0.0015	2.4824
-1.0% D/F	N-fit	1.7510	0.0564	1.8269	0.0477	0.4635	1.337
	FRAKB	1.7577	0.0650	1.8015	0.0337	0.1058	0.6784
	L-fit	1.7588	0.0663	1.8167	0.0421	0.3004	1.0371
+10.0% D/F	N-fit	0.1660	8.2211	0.0010	4.8040	0.0001	10.4400
	FRAKB	0.0819	8.1343	0.0030	4.8051	0.0003	10.4406
	L-fit	0.0744	8.1255	0.0018	4.8044	0.0002	10.4403
-10.0% D/F	N-fit	8.2857	0.0226	15.6493	0.0337	4.8732	0.9217
	FRAKB	8.2904	0.0296	15.6338	0.0227	4.5485	0.2309
	L-fit	8.2912	0.0308	15.6425	0.0289	4.6550	0.4575
+10.0% R	N-fit	0.9456	0.0334	0.0041	0.0483	0.0005	1.4926
	FRAKB	0.9477	0.0362	0.0084	0.0506	0.0013	1.4939
	L-fit	0.9483	0.0368	0.0060	0.0493	0.0008	1.4932
-10.0% R	N-fit	1.1696	0.3129	0.1992	0.1532	0.3881	2.1959
	FRAKB	1.1368	0.2720	0.1900	0.1483	0.4143	2.2434
	L-fit	1.1254	0.2577	0.1928	0.1498	0.6412	2.6551

Figure 4. The Smoker L -fit for example column 2, benzene-toluene.

flow (L_r), and 10% changes to the reflux ratio (R) with a constant D/F . In all cases, except for the -10% R case under example 3, the L -fit method results are closer to the tray-by-tray solutions. This one exception apparently occurs where the error introduced by the simple ratioing of the refluxes has its greatest effect.

Based on the data presented in Table II, a relative percentage error was calculated for each of the approximate solutions. The arithmetic mean and standard deviation of the absolute value of these errors are shown in Table III. These statistics are presented both overall and by individual example column. Based upon the results for the L -fit method, it appears that the Smoker equations can provide good approximate solutions for columns with product impurities down to the 100 parts per million range.

These results are actually quite good except when the product compositions are passing through the "breakthrough" region which occurs near the D/F ratio that results in maximum separation (defined as $x_d - x_b$). For column 1, the breakthrough occurs on the +1.0% case. For column 3, breakthrough occurs on the -1.0% case which

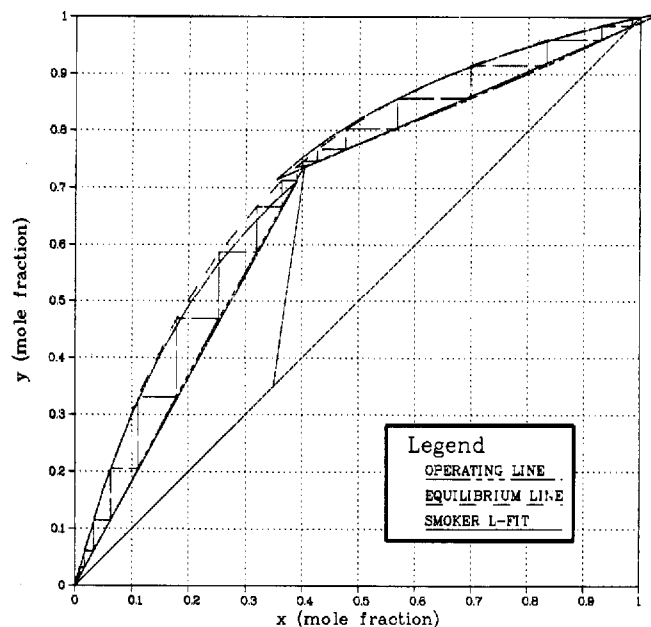
Figure 5. The Smoker L -fit for example column 3, benzene-MCB.

Table III. Analysis of Results Using the Absolute Value of Relative Percentage Error

method	example 1	example 2	example 3	over-all
N-fit,				
mean error,	22.0	24.0	80.0	42.0
std dev	31.0	28.0	117.0	75.0
L-fit,				
mean error,	3.1	14.0	43.0	20.0
std dev	3.3	18.0	53.0	36.0

has the poorest results of all the parametric cases presented. For column 2, the effect is less noticeable since the maximum separation tends to occur near the base case itself. For columns operating in these purity ranges, even 1.0% D/F variations are quite large; however, once the "breakthrough" regions are passed, the approximate solutions again become quite good.

Visual inspection of the McCabe-Thiele diagram and Smoker L -fit should be used on new distillation systems and compared to these samples for qualitative confirmation of the suitability of the method. A poorer fit will

obviously result in worse approximate solutions. Better results can be expected in columns with lower product purities or higher R/R_m ratios.

Multicomponent Distillation

Although these algorithms apply only to binary systems, the solutions may be extended to multicomponent columns by a variety of methods. The most accurate approach is to use individual component distribution coefficients in a manner similar to that proposed by Geddes (1958). This approach requires an additional iterative solution in order to satisfy multicomponent product specifications. Holland and Kuk (1975) describe one such iterative procedure for satisfying the product specifications, and the solution to the Smoker equations could easily be incorporated into their procedure to predict new B/D ratios at alternate conditions.

Another much simpler, but less accurate, approach suggested by Hengstebeck (1961) for approximate solutions is to assume that all components lighter than the light key go overhead and all components heavier than the heavy key go out the bottom of the column. Shinsky (1977) advocates the use of this much simpler approach for column control analysis. Jafarey et al. (1980) also discuss its use in steady-state decoupling analysis.

This latter approach allows the binary solutions to be extended to multiple components explicitly by applying the following equations

$$x_{dl} + x_{dh} = 1 - \frac{F}{D}x_{fl} \quad (14)$$

$$x_{bl} + x_{bh} = 1 - \frac{F}{B}x_{fh} \quad (15)$$

The results obtained using this assumption have been found to fall generally within the accuracy of the Smoker equation assumptions previously examined.

Conclusions

An algorithm for the iterative solution of the Smoker equations to determine implicit operating variables and product compositions in two product, binary distillation columns has been presented. This algorithm provides increased reliability and an order of magnitude improvement in rate of convergence over methods currently described in the literature. The accuracy of these solutions even for nonideal systems has been examined and found to be quite good for columns with product impurities down to the 100 parts per million range. The effects of nonideality, high product purity, and low reflux to minimum reflux ratios are clearly illustrated in the example columns presented.

Because the algorithm is very rapid and reliable, it can easily be used inside other iterative computations such as for relatively accurate multicomponent solution techniques. Furthermore, using the assumption that the heavier than heavy key is negligible in the distillate and that the lighter than light key is negligible in the bottoms results in a very rapid, though more approximate, multicomponent solution technique. This latter technique is well suited for many optimization, reliability, and control studies, and is ideal for fast real-time calculations such as interactive computations and on-line feedforward/decoupling column control using a minicomputer.

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Appendix

The following computational block was used for distillation computations under the FLOWTRAN simulation system: FRAKB—a rigorous tray-by-tray material and energy balance distillation block.

All pure-component physical property data were taken from the FLOWTRAN public data base. The following physical property models were used: vapor pressure by the Antoine equation; vapor fugacity by the Redlich-Kwong equation of state; liquid fugacity by the Redlich-Kwong equation of state with the Poynting correction; liquid activity coefficients from regular solution theory. Additional aspects of the FLOWTRAN simulation systems are described in detail in the text by Seader et al. (1977).

Nomenclature

B = bottom flow
 b = intercept of operating line
 C = intermediate constant
 D = distillate flow
 E = Murphree vapor tray efficiency
 F = feed flow
 G = Smoker reflux to actual external reflux ratio
 K = root of equilibrium curve and operating line
 L = reflux flow
 m = slope of operating line (L/V)
 N = number of equilibrium stages
 q = feed quality
 R = reflux ratio (L_r/D)
 V = vapor flow
 x = liquid mole fraction
 y = vapor mole fraction

Greek Letters

α = relative volatility

Subscripts

b = bottoms
 d = distillate
 f = feed
 h = heavy key
 hh = heavier than heavy key
 i = intermediate
 l = light key
 ll = lighter than light key
 m = minimum
 r = rectifying section
 s = stripping section
 1 = smaller root
 2 = larger root

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