Single Formula for Replacing Smoker Equations in Binary Distillation

R. S. RAMALHO
University of Rochester, Rochester, New York
and
F. M. TILLER
University of Houston, Houston, Texas

Generally in the elementary analytical treatment of binary fractionation under conditions of constant relative volatility and constant molar overflow two equations have been employed separately for calculating the number of plates in the fractionating and stripping sections in the form of the well-known Smoker (2) relations. Since all the variables needed for representing column behavior can be compressed into one formula, the use of two equations may be somewhat misleading.

In the procedure used in this paper formulas for the liquid concentrations x_n and x_m are obtained from solutions of the difference equations representing column behavior in the stripping and enriching sections. The values of x_n and x_m are equated at the feed plate, thereby producing a single equation utilizing the following column parameters:

Feed characterization:
$q,\ F,\ x_F$

Top and bottom products:
$x_D,\ x_W,\ D,\ W$

Column variables:
$M,\ N,\ R$

Two of the ten quantities can be eliminated by using the following overall material balances:

$$F = D + W \qquad (1)$$

$$x_F F = x_D D + x_W W \qquad (2)$$

Any analytical equations representing column behavior must contain eight of the variables. For example if D and W are eliminated, the functional relationship could be represented by

$$f(q, F, x_F, x_D, x_W, M, N, R) = 0 \qquad (3)$$

If the feed parameters, reflux, and product compositions are fixed, Equation (3) would reduce to

$$f(M, N) = 0 \qquad (4)$$

Thus the ordinary design problem reduces to an equation giving M as a function of N. Although an infinite number of solutions are possible, the solution for which $(M + N)$ is a minimum corresponds approximately to the result obtained from Smoker's equation.

The difference equations representing material balances in the case of fractionation of a binary mixture can be written as follows:

$$y_{n+1} = \frac{R}{R+1}\, x_n + \frac{x_D}{R+1} \qquad (6)$$

$$y_m = \frac{RD}{RD + qF - W}\, x_{m+1} - \frac{W x_W}{RD + qF - W} \qquad (7)$$

Assuming that equilibrium exists on each plate and that the relative volatility is constant, one can relate x and y by

$$y = \frac{\alpha x}{(\alpha - 1)\, x + 1} \qquad (8)$$

Eliminating y in (6) and (7) and transforming the resulting formulas into Ricatti difference Equations (1, 3) one gets the following solutions:

$$\frac{1}{x_n - \frac{1}{2}(A - B + S)} = \left[\frac{1}{x_D - \frac{1}{2}(A - B + S)} + \frac{1}{S}\right] \left(\frac{A - B + S}{A - B - S}\right)^n - \frac{1}{S} \qquad (9)$$

$$\frac{1}{x_m - \frac{1}{2}(B - A' + S')} = \left[\frac{1}{x_W - \frac{1}{2}(B - A' + S')} + \frac{1}{S'}\right] \left(\frac{B - A' + S'}{B - A' - S'}\right)^m - \frac{1}{S'} \qquad (10)$$

where

$$A = \left(\frac{\alpha}{\alpha - 1}\right) \left(\frac{R + 1}{R}\right) - \frac{x_D}{R}$$

$$A' = \left(\frac{1}{\alpha - 1}\right) \left(\frac{RD + qF - W}{RD - qF}\right) + \frac{W x_W}{RD + qF}$$

$$B = \frac{1}{\alpha - 1}$$

$$S = \sqrt{(A - B)^2 - \frac{4 x_D}{R(\alpha - 1)}}$$

$$S' = \sqrt{(A' - B)^2 - \frac{4 W x_W}{(RD + qF)(\alpha - 1)}}$$

Equations (9) and (10) can be combined to give a single functional relationship between the tower variables. The concentration on the feed plate is given both by x_N and x_M (and not by x_F). Placing $n = N$ and $m = M$ in (9) and (10), solving for x_N and x_M, and equating the results one obtains

$$\frac{1}{\left[\frac{1}{x_D - \frac{1}{2}(A - B + S)} + \frac{1}{S}\right] \left(\frac{A - B + S}{A + B - S}\right)^N - \frac{1}{S}} + \frac{1}{2}(A - B + S) = \frac{1}{\left[\frac{1}{x_W - \frac{1}{2}(B - A' + S')} + \frac{1}{S'}\right] \left(\frac{B - A' + S'}{B - A' - S'}\right)^M - \frac{1}{S'}} + \frac{1}{2}(B - A' + S') \qquad (11)$$

This equation can be manipulated into form

$$\frac{S\left(C - \frac{1}{2}S\right)}{\left(C + \frac{1}{2}S\right) J^N - \left(C - \frac{1}{2}S\right)}$$

$$-\frac{S'\left(C'-\frac{1}{2}S'\right)}{\left(C'+\frac{1}{2}S'\right)K^{M}-\left(C'+\frac{1}{2}S'\right)}+\frac{1}{2}\left(A+A'-2B+S-S'\right)=0 \qquad (12)$$

where

$$C = x_D - \frac{1}{2}(A - B)$$

$$C' = x_W - \frac{1}{2}(B - A)$$

$$J = \frac{A - B + S}{A - B - S}$$

$$K = \frac{B - A' + S'}{B - A' - S'}$$

Equation (12) represents the desired formulation of a single equation representing two component tower behavior.

In general formulas like Equation (12) are desired for every type of stage-by-stage operating involving reflux, whether it be in multicomponent distillation, solvent extraction, or combined absorption and stripping operations. While the number of cases in which an explicit equation like (12) can be obtained are limited, the general philosophy of aiming at such a goal is important.

NOTATION

A, A', B, C, J, K, S, S' = constants defined in paper
D, F, W = distillate, feed, bottoms, moles/hr.
m = plate number measuring up from bottom of tower
M = total number of theoretical plates in stripping section
n = plate number measuring down from condenser
N = total number of theoretical plates in fractionation section
q = ratio of total heat needed to convert 1 mole of feed into saturated vapor to molal latent heat of feed
R = reflux ratio
x, y = liquid and vapor concentrations, mole fraction

Subscripts

D, F, W = distillate, feed, and bottom
m, n = composition on mth and nth plates
α = relative volatility

LITERATURE CITED

1. Ramalho, R. S., M.S. thesis, Vanderbilt Univ., Nashville, Tennessee (1949).
2. Smoker, E. H., *Trans. Am. Inst. Chem. Engrs.*, 34, 456 (1938).
3. Tiller, F. M., and R. S. Tour, *ibid.*, 40, 317 (1944).

INFORMATION RETRIEVAL*

Key Words: A. Reduction-8, Iron Oxide-1, Hematite-1, Magnetite-1, Iron Oxide-2, Iron-2, Hydrogen-5, Iron Oxide Spheres-6, Temperature-6, Residence Time-6, Reduction-7, Electron-Micrographs-7, Reactors-10. B. Gas-Conveyed Reactions-8, Design-8, Reactors-9.

Abstract: The reduction of iron oxide spheres in hydrogen was studied by means of the atomized suspension technique, in which a dilute suspension of the oxide particles is conveyed by the reducing medium through a reactor, the walls of which are maintained at an elevated temperature.

The rate of the reaction was studied as a function of particle diameter (5 to 100 μ), residence time (2 to 13 sec.) and temperature (500° to 1100°C.). For particles above 40 μ the results were correlated by a rate equation based on the analysis of data of twelve other investigations, and the proposed mechanism was supported by electron-photomicrographs of the reduced spheres.

Reference: Themelis, N. J., and W. H. Gauvin, **A.I.Ch.E. Journal, 8,** No. 4, p. 437 (September, 1962).

Key Words: Filtration-8, Local Porosity-7, Hydraulic Pressure-7, Average Porosity-7, Total Pressure-6, Distance Through Solid-6, Theoretical Analysis-1.

Abstract: Equations are derived for porosity and hydraulic pressure variation in filter cakes. Numerical methods and empirical equations are developed. Average porosity is presented as a function of total pressure. Slope of porosity vs. distance curves are shown to be widely different for various substances.

Reference: Tiller, F. M., and Harrison Cooper, **A.I.Ch.E. Journal, 8,** No. 4, p. 445 (September, 1962).

Key Words: Decomposition-9, Cracking (Chemical)-9, Rates-9, Reactions-9, Kinetics-9, Reaction Kinetics-9, Reaction Mechanics-9, Distribution-8, Temperature-8, Residence-8, Time-8, Profiles-8, Diffusion-8, Activation-8, Energy-, Methane-1, Hydrocarbons-1, Ammonia-1, Heat Transfer-6, Feed-6, Rates-6, Conversion-7, Jets-10, Plasma-10, Models-10, Tubes-10, Reactors-10, Flow-.

Abstract: Study of the decomposition of ammonia and methane in a tube confined plasma jet shows the rates and the activation energies for the two reactions to be nearly identical and much too low to be limited by dissociation processes. An approximate model is set up for the diffusion of reagent gas into the plasma as the rate limiting step, and it is found to agree well with the measured degree of conversion as a function of heat flow and reagent feed rate. This model is then extended to examine its implications in terms of various parameters of interest.

Reference: Freeman, M. P., and J. F. Skrivan, **A.I.Ch.E. Journal, 8,** No. 4, p. 450 (September, 1962).

Key Words: A. Equilibrium-8, Distillation-9, IBM-650-10, Computer-10, Activity Coefficient-7, Internal Pressure-6, Polar Internal Pressure-6, Nonpolar Internal Pressure-6, Liquid Volume-6, Temperature-6, Solution Theory-8, Binary-, Azeotropic-, Extractive-, Solvent-4, Vapor-5, Liquid-5, van Laar-, van Arkel-, Scatchard-, Hildebrand-, van Laar Constants-7. B. Internal Pressure-7, Pressure-6, Temperature-6, Compressibility Factor-6, Vapor Pressure Slope-6, Critical-, Reduced-, Theorem of Corresponding States-10, Reidel-, Lyderson-.

Abstract: This method for predicting the vapor liquid equilibrium for polar-nonpolar binary systems is based upon the van Arkel modification of the Scatchard-Hildebrand equations which utilize the concept of internal pressure. A method of predicting the apparent internal pressure based upon the theorem of corresponding states is presented. The method helps in finding suitable solvents for azeotropic and extractive distillation.

Reference: Finch, R. N., and Matthew Van Winkle, **A.I.Ch.E. Journal, 8,** No. 4, p. 455 (September, 1962).

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[*] For details on the use of these key words and the A.I.Ch.E. Information Retrieval Program, see **Chem. Eng. Progr., 57,** No. 5, p. 55 (May, 1961), No. 6, p. 73 (June, 1961).

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