

Batch Distillation: Abbreviated Theory

In order to separate the components of a liquid mixture by distillation, one takes advantage of the equilibrium between the vapor and liquid phases. For an ideal binary solution, Raoult's law applies:

$$P_A = P_A^* x_A \quad (1a)$$

$$P_B = P_B^* x_B \quad (1b)$$

where P_A and P_B are the partial pressures, x_A and x_B are the mole fractions in the liquid phase, and P_A^* and P_B^* are the pure component vapor pressures. Also, if the vapor phase is ideal:

$$P_T = P_A + P_B \quad (2)$$

where P_T is the total pressure.

Some mixtures show positive deviations from Raoult's law and form minimum boiling azeotropes. An example is the 1-propanol-water mixture. Some mixtures show negative deviations and form maximum boiling azeotropes.

Two methods are commonly used for distillation calculations. The method of Ponchon and Savarit requires detailed enthalpy data, while the method of McCabe and Thiele requires only concentration equilibrium data. The method of McCabe and Thiele involves performing material balances around each section of the column. Here the n^{th} section includes the top of the column and all stages (plates) counting downward to stage n (see Fig. 1). A total material balance on section n gives:

$$V_{n+1} = L_n + D \quad (3)$$

and a balance on a particular component gives:

$$V_{n+1} y_{n+1} = L_n x_n + D x_D \quad (4)$$

where V_i is the molar flow rate of vapor from stage i , L_i is the molar flow rate of liquid from stage i , D is the molar flow rate of distillate from the top of the column (assumed to be totally condensed), y_i is the mole fraction of the particular component in the vapor leaving stage i and x_i

is the mole fraction of the particular component in the liquid leaving stage i . The reflux ratio, R , is then defined as

$$R = \frac{L_o}{D} \quad (5)$$

where L_o is the molar flow rate of the reflux stream. Substituting this definition into equation (4) and rearranging gives

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

Equation (6) is known as the operating line. At total reflux ($D \rightarrow 0$; $R \rightarrow \infty$), the operating line coincides with the 45° line on a plot of y vs. x . This operating line and the vapor-liquid equilibrium curve can be plotted on an x - y axis, and the McCabe-Thiele method used to find the minimum number of theoretical stages. A real column typically won't work quite this well, so an efficiency can be calculated using equation (7).

$$E = \frac{\text{number of equilibrium stages calculated}}{\text{number of actual stages required}} \quad (7)$$

Here are a few other references where you can learn more of the details.

1. Treybal, R.E.: "Mass Transfer Operations," 2nd Edition, McGraw-Hill, 1968.
2. Foust, A.L. et al., "Principles of Unit Operations," Wiley, New York, 1960.
3. Jimmerrmans, J.: "The Physico-Chemical Constants of Binary Systems in Concentrated Solutions," Vol. 4, Interscience Publishers, Inc.