Maximum Separation in Binary and Multicomponent Flash Operations

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Introduction

The flash operation is a well-known process in vapor-liquid separation technology. It is a common industrial practice (Mansouri, 1979) and a basic precursor to the teaching of staged distillation. Flash calculations are routine in most material and energy balance simulator packages and other computer methods (Kinoshita and Takamatsu, 1986). Flash calculations can arise in various processes (Morozova et al., 1974; Elliot, 1976) and in multiphase flow situations (Shock, 1976).

The flash operation itself is shown in Figure 1, which is the well-known textbook representation (Wankat, 1988) for setting up material balances and heat balances between input feed (F) and the flash product streams (V and L). Once the equilibrium relationship, $y_i = f(x_i)$, is determined, the equations below can be solved for V/L split and output compositions, assuming fixed temperature and pressure in the flash drum:

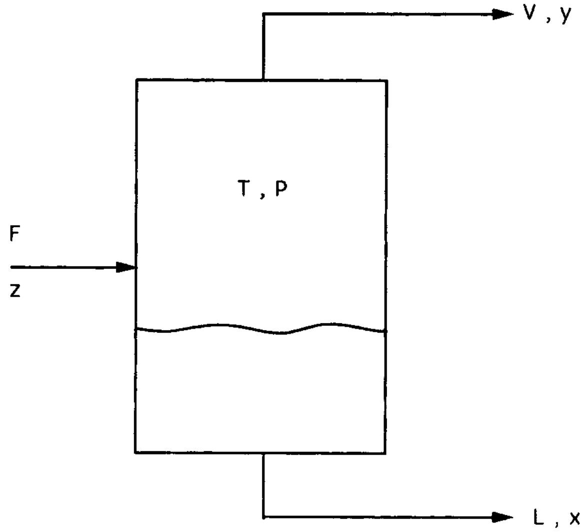

Figure 1. Equilibrium flash separation.

$$F = V + L \tag{1}$$

$$z_i F = y_i V + x_i L \tag{2}$$

$$y_i = f(x_i) \tag{3}$$

At one extreme, the largest value of y_i for the lightest component is obtained at the bubble point, where V is infinitesimally small. At the other extreme, the largest recovery of component (in the vapor) occurs at the dew point, where V is equal to F, and L is zero. Neither extreme involves a *separation* of the feed, which all goes to liquid in the first case or vapor in the second.

Separation is obtained in a flash operation by specifying the pressure and temperature in the flash drum, so that the temperature is between the two extremes mentioned above. Depending on exactly where that temperature is set, various splits will occur. These principles apply equally to binary and multicomponent flash operations.

Theory

To recommend maximum separation conditions, a maximizing function must be found. It cannot be V or V/F, y or y/x, relative volatility, or a host of other commonly known variables or combinations, because these functions do not have maxima between bubble and dew points, necessarily. The functions yV/zF or yV/xL always maximize at $V/F = 1$, the dew point. Thus, they too are unsuitable. The relative volatility is often recommended as a separation factor, but this does not work well here. It will maximize at the extremes, depending on the equilibrium characteristics, and will not maximize at all for constant relative volatility systems.

The maximizing function must contain a relationship both to the composition and to the total mass. A suitable maximizing function may be defined as:

$$f = \left(\frac{V}{F}\right)\left(\frac{y-z}{z}\right) \tag{4}$$

which can be derived from the following considerations:

$$f=(V/F)[(y-y_{dew})/(y_{bubl}-y_{dew})]=(A)(B) \tag{5}$$

where A is the fraction vaporized (a total mass or moles relation), and B is the normalized vapor composition relative to the dew point. Since $y_{dew}=z_i$, and $y_{bubl}=K_{bubl}z_i$ (where K_{bubl} is a constant known from pressure and the bubble point temperature):

$$f=(V/F)[(y-z)/(K-1)z] \tag{6}$$

The $K-1$ term is a constant that affects only the absolute value of f, not the maximum, and can therefore be omitted; the simplest form, Eq. 4, then results.

That this function must have a maximum (or a minimum) can be shown by the following: at the dew point, $V/F=1$, but $(y-z)/z=0$, and $f=0$. At the bubble point, the opposite occurs: $V/F=0$, and $(y-z)/z$ is the highest value it can reach. Thus, if V/F goes to zero at the bubble point, and if $(y-z)/z$ goes to zero at the dew point, a maximum (or a minimum, depending on equilibrium relationships) must exist in-between. Several examples are shown to illustrate the use of this maximizable function, f.

The function can be generalized to include maximizing a "cut" or group of k components in an n-component flash separation by summing on the component of interest and, for example, those lighter ($k-1$ components). Then,

$$f=(V/F)\left(\sum_1^k y_i-\sum_1^k z_i\right)\Big/\sum_1^k z_i \tag{7}$$

The conditions of the maximum defined by Eq. 7 will not, in all likelihood, be the same as any one component, but rather the group as defined by the user.

Results and Discussion

In the following examples, iterative procedures are used to calculate either or both parts of the maximizing function, f. This is necessary because the equilibrium and operating (mass balance) relations are implicit and cannot be extracted with closed-form equations. A computer is useful, but not necessary, for the iterative procedures. A graphical approach is particularly suitable for the binary method, but the function, f, must still be plotted before the maximum can be found. This can be done by eye or by some numerical technique using the function points.

Binary example

The ethanol-water T-x-y diagram at 1-atm pressure is shown in Figure 2, along with an example of one step in the solution algorithm. The feed composition is 12 mol % ethanol.

The algorithm is:

a) Obtain the equilibrium data (T-x-y) at a given pressure.

b) Fix the feed line and bubble and dew point temperatures.

c) Choose a temperature along the feed line between bubble and dew points. Obtain x,y compositions and fraction vaporized, V/F, by inverse lever-arm rule or material balance equations.

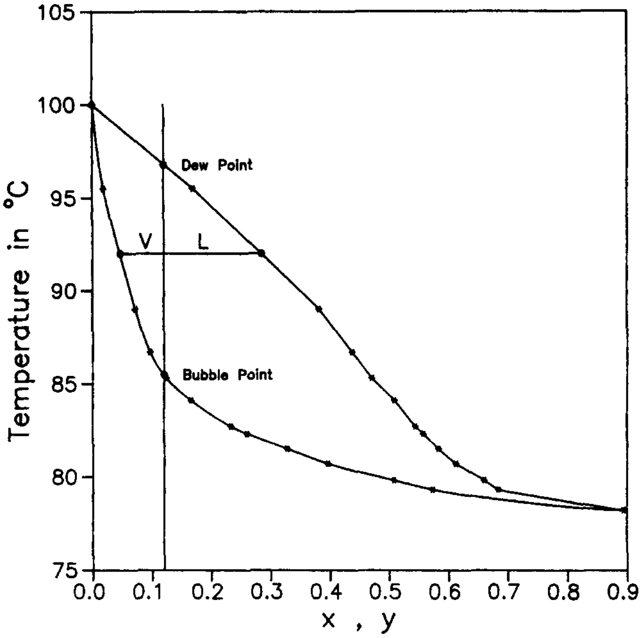

Figure 2. Ethanol-water system, calculating parameters for flash optimization.

d) Use information of (c) to calculate f according to Eq. 4.

e) Repeat for different temperatures so that the function f can be plotted against the temperature. Find the maximum.

Figure 3 shows the results, where the function f has a maximum at 92°C. This will give the most separation of ethanol between the vapor and feed streams. These conditions correspond to a recovery of 82.1% in the vapor stream.

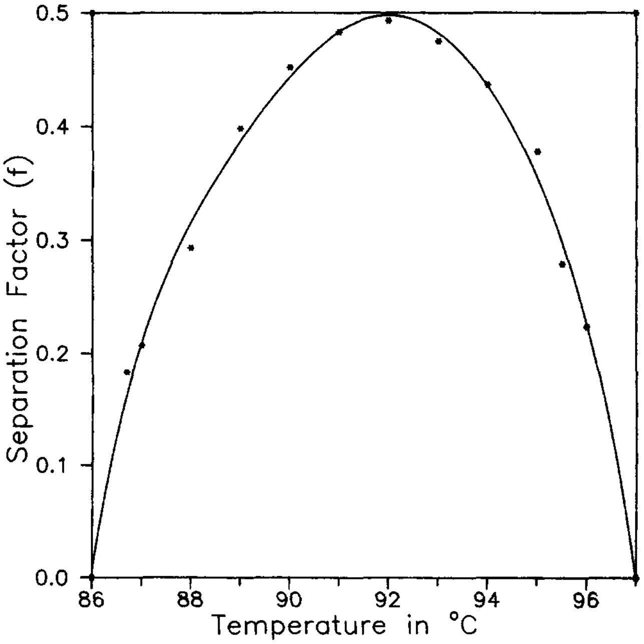

Figure 3. Ethanol-water system, maxima in optimum recovery function depending on temperature.

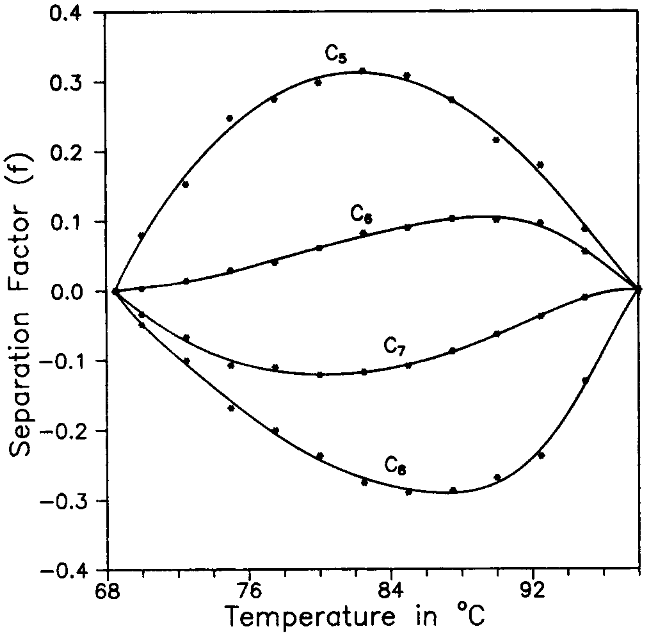

Figure 4. Multicomponent example 1, maxima in optimum recovery function depending on temperature.

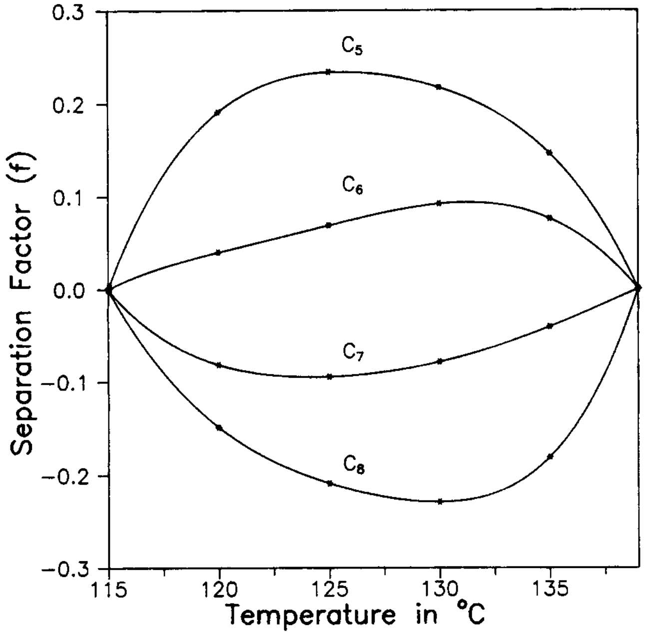

Figure 6. Multicomponent example 2, maxima in optimum recovery function depending on temperature at 3 atm.

Multicomponent example 1

For this example, a typical hydrocarbon feed consisting of equal amounts of *n*-pentane, *n*-hexane, *n*-heptane and *n*-octane (C_5-C_8) at 1 atm is used. The DePriester chart equilibrium K-value data, alternative graphical representations thereof (Eq. 7), or equations describing these data may also be used. For this mixture, the bubble point was 68.5°C, and the dew point was 98°C, calculated by standard trial-and-error methods (Wankat, 1988; McCabe et al., 1985). By fixing temperatures in-between dew and bubble points, the K's can be readily obtained and the y_i's calculated. The fraction vaporized must be calculated by the Rachford-Rice equation, which cannot be solved explicitly. Well-known numerical techniques, such as Newton's method, secant method, or the like, can be employed for its solution (Wankat, 1988). This must be done for every temperature selected between bubble and dew points. The function f can then be easily calculated from the V/F of the Rachford-Rice equation and the y_i from equilibrium data.

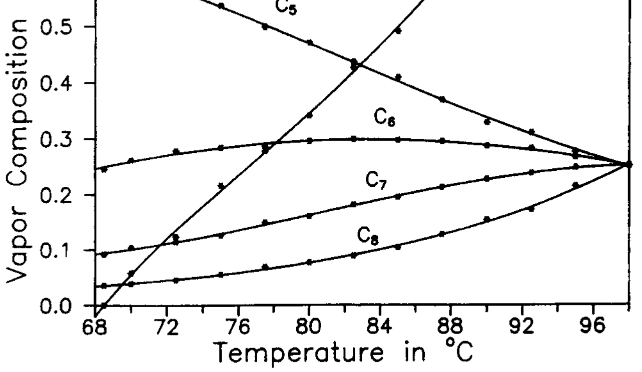

Figure 5. Multicomponent example 1, vapor compositions and fraction vaporized as a function of flash temperature at 1 atm.

Figure 4 shows the results for this example. Two components show maxima, and two show minima; but all these occur at different temperatures. As expected, the most volatile component has the largest maximum, and the least volatile has the largest minimum. From Figure 4, a temperature almost midway between bubble and dew points will maximize the separation for the lightest component (C_5), but not the others.

Figure 5 shows the V/F and y_i data as a function of temperature. As is typical, the V/F function is a continuously increasing curve with a mild S-shape. The vapor composition of the lightest component continuously decreases with temperature. The two heaviest components show increasing vapor composition with temperature, and the C_6 component shows a broad maximum.

Multicomponent example 2 (pressure)

The identical multicomponent mixture as in example 1 was used at 3-atm flash pressure for this example to show the effect of pressure on the maxima. The same procedures were employed. Figure 6 shows these results. The bubble point-dew point envelope changes, and the maxima seem to be squeezed

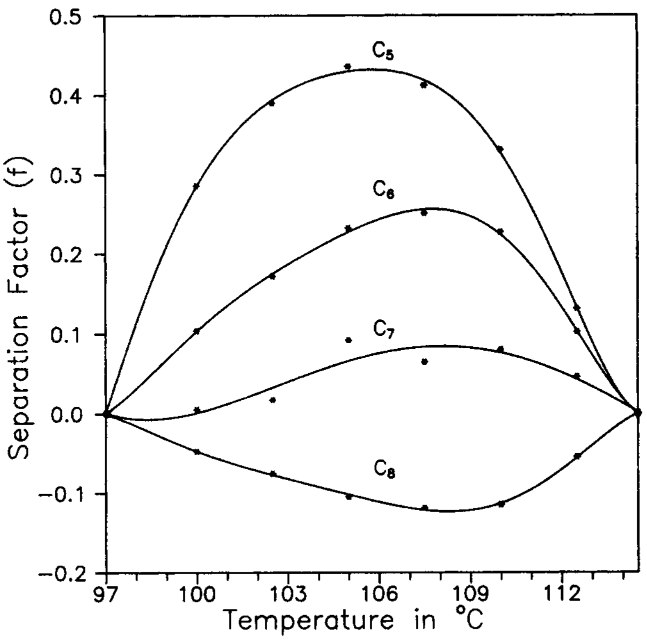

Figure 7. Multicomponent example 3, maxima in optimum recovery function depending on temperature at 1 atm with different feed composition.

closer together and occur at relatively lower temperatures in the envelope.

Multicomponent example 3 (composition)

This example is presented to show that these results depend on feed composition. In this example, the pressure is 1 atm again, but the feed composition was changed to $C_5 = 0.05$, $C_6 = 0.10$, $C_7 = 0.30$, and $C_8 = 0.55$. The same procedures were used once again, and the results are shown in Figure 7. Here, there are three maxima, not two as before, but similar behavior is shown. The maximum seems to shift to lower temperatures for lighter components, but a distinctly different temperature is associated with maximizing the separation of a particular component.

Generalized function

Equation 7 can be used to maximize the recovery of a "cut" or group of components. This is illustrated using the conditions of example 1. If the cut comprising C_5 and C_6 components together is to be maximized, the use of Eq. 7 gives a curve similar to both C_5 and C_6 curves in Figure 4, but the maximum is at a temperature (106.5°C) which is in-between the maximizing conditions for either component. (In general, simultaneous maximum recovery of multiple components is not possible, except fortuitously.) The temperature that maximizes the "cut" recovery is closer to the C_6 optimum condition, because there is relatively more C_6 than C_5.

Conclusions

A maximizing function has been defined, and procedures have been developed for both binary and multicomponent flash operations, whereby the maximum separation of component can be obtained. In general, the temperature condition of the maximum will differ for each component so that setting the flash at one temperature will not maximize the recovery of every component in the multicomponent mixture. A generalized form of the maximizing function can be used to obtain maximum recovery of a "cut" or group of components defined by the user, for example, light key plus all components lighter.

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