11.6.4. Batch or continuous distillation

A discussion on the relative merits of batch and continuous distillation is given by ELLIS[36], who shows that when a large number of plates is used and the reflux ratio approaches the minimum value, then continuous distillation has the lowest reflux requirement and hence operating costs. If a smaller number of plates is used and high purity product is not required, then batch distillation is probably more attractive.

11.7. MULTICOMPONENT MIXTURES

11.7.1. Equilibrium data

For a binary mixture under constant pressure conditions the vapour–liquid equilibrium curve for either component is unique so that, if the concentration of either component is known in the liquid phase, the compositions of the liquid and of the vapour are fixed. It is on the basis of this single equilibrium curve that the McCabe–Thiele method was developed for the rapid determination of the number of theoretical plates required for a given separation. With a ternary system the conditions of equilibrium are more complex, for at constant pressure the mole fraction of two of the components in the liquid phase must be given before the composition of the vapour in equilibrium can be determined, even for an ideal system. Thus, the mole fraction y_A in the vapour depends not only on x_A in the liquid, but also on the relative proportions of the other two components.

Determining the equilibrium relationships for a multicomponent mixture experimentally requires a considerable quantity of data, and one of two methods of simplification is usually adopted. For many systems, particularly those consisting of chemically similar substances, the relative volatilities of the components remain constant over a wide range of temperature and composition. This is illustrated in Table 11.2 for mixtures of phenol, ortho and meta-cresols, and xylenols, where the volatilities are shown relative to ortho-cresol.

Table 11.2.   Volatilities relative to o-cresol

	Temperature (K)		
	353	393	453
phenol	1.25	1.25	1.25
o-cresol	1	1	1
m-cresol	0.57	0.62	0.70
xylenols	0.30	0.38	0.42

An alternative method, particularly useful for the separation of multicomponent mixtures of hydrocarbons, is to use the simple relation $y_A = Kx_A$. K values have been measured for a wide range of hydrocarbons at various pressures, and some values are shown in Figure 11.39.

Some progress has been made in presenting methods for calculating ternary data from known data for the binary mixtures, though as yet no entirely satisfactory method is available.
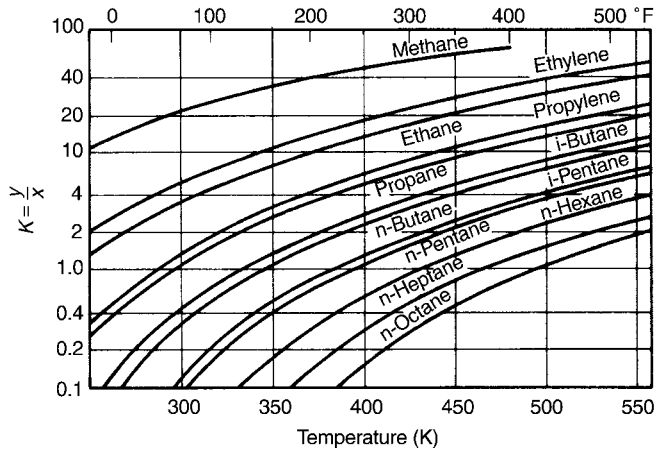
Figure 11.39.   Vapour−liquid equilibrium data for hydrocarbons

11.7.2. Feed and product compositions

With a binary system, if the feed composition x_f and the top product composition x_d are known for one component, then the composition of the bottoms x_w may have any desired value, and a material balance will determine the amounts of the top and bottom products D and W. This freedom of selecting the compositions does not apply for mixtures with three or more components. GILLILAND and REED[37] have determined the number of degrees of freedom for the continuous distillation of a multicomponent mixture. For the common case in which the feed composition, nature of the feed, and operating pressure are given, there remain only four variables that may be selected. If the reflux ratio R is fixed and the number of plates above and below the feed plate are chosen to give the best use of the plates, then only two variables remain. The complete composition of neither the top nor bottom product can then be fixed at will. This means that some degree of trial and error is unavoidable in calculating the number of plates required for any desired separation. Thus, if a trial composition is taken, and it is found that for the given bottom composition the desired top composition is not obtained with the selected reflux ratio, then an adjustment must be made in the bottom composition. An exact fit in a calculation of this kind is not essential since the equilibrium data and the plate efficiency are known with only limited accuracy. This problem is frequently simplified if a sharp cut is to be made between the components, so that all of the more volatile components appear in the top and all of the less volatile in the bottom product.

11.7.3. Light and heavy key components

In the fractionation of multicomponent mixtures, the essential requirement is often the separation of two components. Such components are called the key components and by concentrating attention on these it is possible to simplify the handling of complex mixtures. If a four-component mixture **A**−**B**−**C**−**D**, in which **A** is the most volatile and **D** the least volatile, is to be separated as shown in Table 11.3, then **B** is the lightest component appearing in the bottoms and is termed the light key component. **C** is the

Table 11.3.   Separation of multicomponent mixture

Feed	Top product	Bottoms
A	**A**	
B	**B**	**B**
C	**C**	**C**
D		**D**

heaviest component appearing in the distillate and is called the heavy key component. The main purpose of the fractionation is the separation of **B** from **C**.

11.7.4. The calculation of the number of plates required for a given separation

One of the most successful methods for calculating the number of plates necessary for a given separation is due to LEWIS and MATHESON[38]. This is based on the Lewis–Sorel method, described previously for binary mixtures. If the composition of the liquid on any plate is known, then the composition of the vapour in equilibrium is calculated from a knowledge of the vapour pressures or relative volatilities of the individual components. The composition of the liquid on the plate above is then found by using an operating equation, as for binary mixtures, although in this case there will be a separate equation for each component.

If a mixture of components **A**, **B**, **C**, **D**, and so on has mole fractions x_A, x_B, x_C, x_D, and so on in the liquid and y_A, y_B, y_C, y_D, and so on in the vapour, then:

$$y_A + y_B + y_C + y_D + \cdots = 1 \tag{11.104}$$

and:

$$\frac{y_A}{y_B} + \frac{y_B}{y_B} + \frac{y_C}{y_B} + \frac{y_D}{y_B} + \cdots = \frac{1}{y_B}$$

$$\alpha_{AB}\frac{x_A}{x_B} + \alpha_{BB}\frac{x_B}{x_B} + \alpha_{CB}\frac{x_C}{x_B} + \alpha_{DB}\frac{x_D}{x_B} + \cdots = \frac{1}{y_B}$$

$$\Sigma(\alpha_{AB}x_A) = \frac{x_B}{y_B} \tag{11.105}$$

$$y_B = \frac{x_B}{\Sigma(\alpha_{AB}x_A)} \tag{11.106}$$

and, similarly: $y_A = \dfrac{x_A\alpha_{AB}}{\Sigma(\alpha_{AB}x_A)}; \quad y_C = \dfrac{x_C\alpha_{CB}}{\Sigma(\alpha_{AB}x_A)}; \quad y_D = \dfrac{x_D\alpha_{DB}}{\Sigma(\alpha_{AB}x_A)}$ (11.107)

Thus, the composition of the vapour is conveniently found from that of the liquid by use of the relative volatilities of the components. Examples 11.14–11.17 which follow illustrate typical calculations using multicomponent systems. Such solutions are now computerised, as discussed further in Volume 6.

Example 11.14

A mixture of ortho, meta, and para-mononitrotoluenes containing 60, 4, and 36 mole per cent respectively of the three isomers is to be continuously distilled to give a top product of 98 mole