

Chapter 2:

Flash Distillation

Flash distillation can be considered one of the *simplest* separation processes

In this process, a pressurised *feed stream*, which is in *liquid phase*, is passed through a throttling valve/nozzle or an expansion valve/nozzle (sometimes, the feed stream may be passed through a heater before being passed through the valve/nozzle, in order to pre-heat the feed) connected to a tank or drum, which is called a “*flash*” tank or drum

After being passed through the valve/nozzle, the feed enters the tank/drum, whose pressure is low; thus, there is a substantial pressure drop in the feed stream, causing the feed to *partially* vaporise

The fraction that becomes *vapour goes up* to and is *taken off* at the ***top*** of the tank/drum

The remaining *liquid part goes down* to and is *withdrawn* at the ***bottom*** of the tank/drum

It is noteworthy that, although the illustration (Figure 2.1) of the flash tank is in *vertical* direction (แนวตั้ง), *flash tanks/drums* in *horizontal* direction (แนวนอน) are also *common*

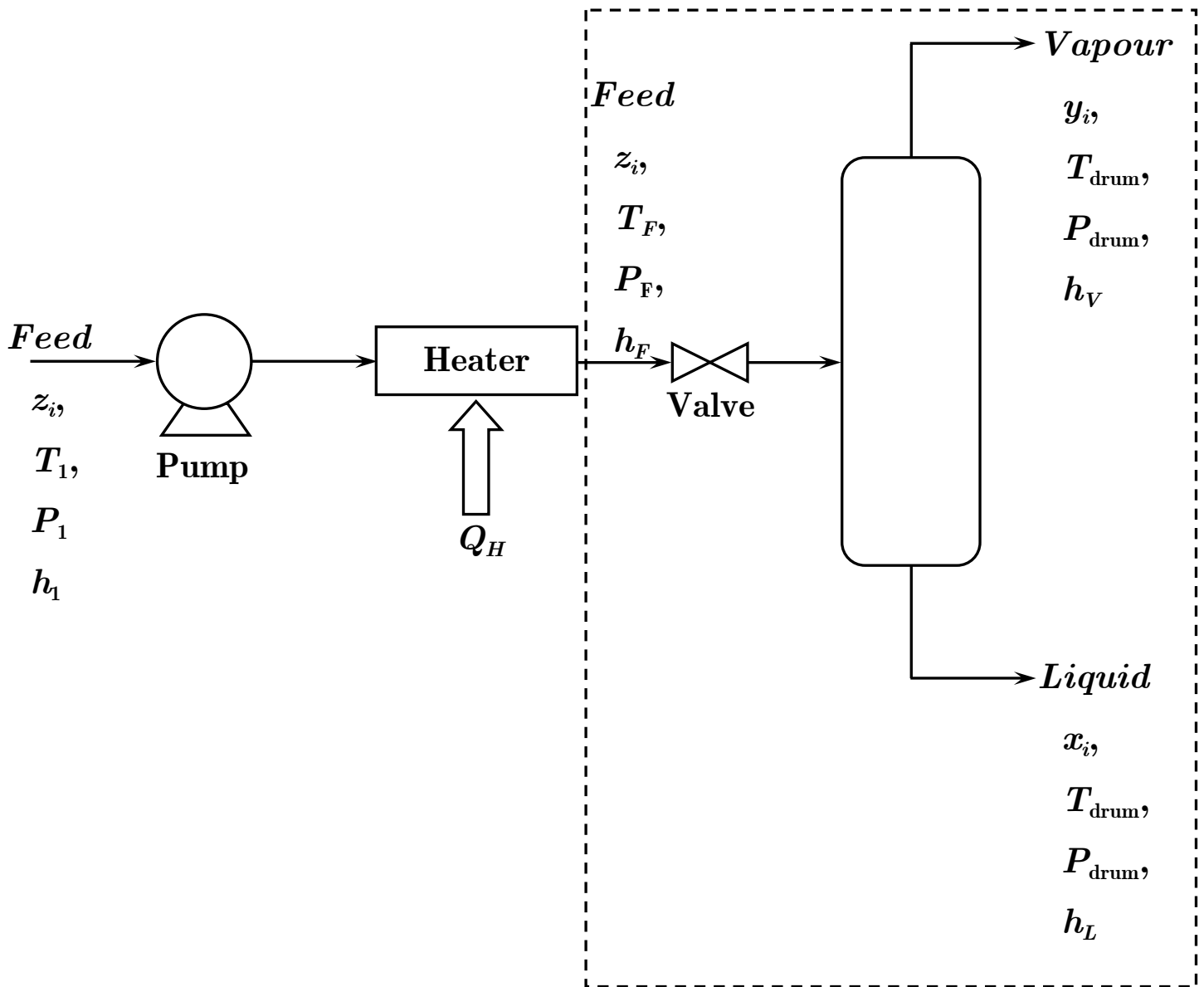


Figure 2.1: A flash distillation system

Let's denote the amount (in mole) of

- feed as F
- liquid fraction as L
- vapour fraction as V

The overall material (or mole) balance for the system within the dashed boundary can be written as follows

$$F = L + V \quad (2.1)$$

Species balance (for species i) can also be performed as follows

$$z_i F = x_i L + y_i V \quad (2.2)$$

The energy balance for this system is

$$Fh_F + Q_{\text{Flash}} = Lh_L + Vh_V \quad (2.3)$$

Commonly, $Q_{\text{Flash}} = 0$, or nearly 0, as the flash distillation is usually operated *adiabatically*

Thus, Eq. 2.3 can be reduced to

$$Fh_F = Lh_L + Vh_V \quad (2.4)$$

To determine the amount of Q_H (or to determine the size of the heater), an energy balance around the heater is performed as follows

$$Fh_1 + Q_H = Fh_F \quad (2.5)$$

It should be noted that, if the feed contains only 2 components (*i.e.* the feed is a *binary* mixture), it results in the following facts:

- Before being fed into the tank, the feed contains only one phase (*i.e.* liquid phase); thus the degree of freedom is

$$\begin{aligned} F &= C - P + 2 \\ &= 2 - 1 + 2 \end{aligned}$$

$$F = 3$$

[note that F = degree of freedom, C = number (#) of species, and P = number (#) of phases]

- After being fed into the tank, the feed is divided into 2 phases (*i.e.* liquid and vapour phases), which results in the degree of freedom of

$$\begin{aligned} F &= C - P + 2 \\ &= 2 - 2 + 2 \end{aligned}$$

$$F = 2$$

This means that

- before the feed is being fed into the tank, it requires 3 variables (*e.g.*, z , T , and P) to identify other properties of the system (*e.g.*, h , s)
- after the feed is passed into the tank, it requires only 2 variables (*e.g.*, x_i and P_{drum} or y_i and T_{drum}) to obtain exact values of other properties

2.1 Equilibrium data

In principle, equilibrium data of liquid and vapour (generally called vapour-liquid equilibrium: VLE) can be obtained experimentally

Consider a chamber containing liquid and vapour of a mixture (*i.e.* there are more than one species) at specified temperature (T) and pressure (P) where both phases are allowed to be settled, meaning that the *liquid* and *vapour* phases are *in equilibrium* with each other (Figure 2.2)

After the system reaches the equilibrium, each of liquid and vapour phases is sampled and then analysed for its composition

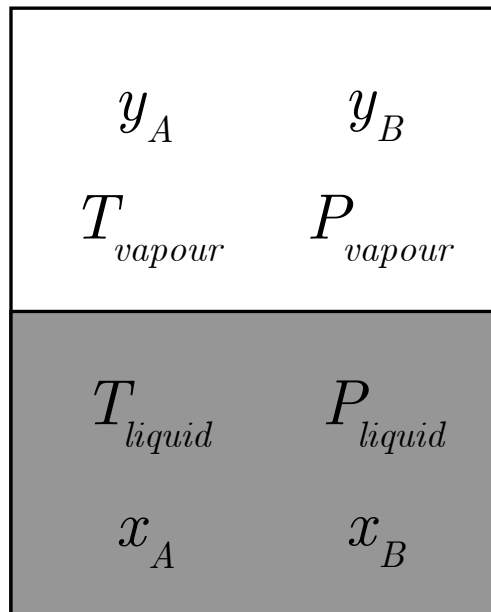


Figure 2.2: An example of vapour-liquid equilibrium (VLE)

Normally, the *experiment* can be *conducted* in either *constant pressure* (where the system's temperature is varied) or *constant temperature* (where the pressure of the system is varied) mode

Table 2.1 illustrates the equilibrium data for various temperatures of the system containing ethanol (EtOH: E) and water (W) at the pressure of 101.3 kPa (or 1 atm)

Note that, as this is a *binary* mixture, at any specified temperature (or pressure), we obtain the facts that

$$x_E = 1 - x_W$$

and

$$y_E = 1 - y_W$$

Table 2.1: VLE data for an EtOH-water binary mixture at 1 atm

T (°C)	x_E	x_W	y_E	y_W
100	0	1.0000	0	1.0000
95.5	0.0190	0.9810	0.17	0.8300
89.0	0.0721	0.9279	0.3891	0.6109
86.7	0.0966	0.9034	0.4375	0.5625
85.3	0.1238	0.8762	0.4704	0.5296
84.1	0.1661	0.8339	0.5089	0.4911
82.7	0.2337	0.7663	0.5445	0.4555
82.3	0.2608	0.7392	0.558	0.4420
81.5	0.3273	0.6727	0.5826	0.4174
80.7	0.3965	0.6035	0.6122	0.3878
79.7	0.5198	0.4802	0.6599	0.3401
79.3	0.5732	0.4268	0.6841	0.3159
78.7	0.6763	0.3237	0.7385	0.2615
78.4	0.7472	0.2528	0.7815	0.2185
78.2	0.8943	0.1057	0.8943	0.1057
78.3	1.0000	0	1.0000	0

The *VLE data* in Table 2.1 can also be presented *graphically* as

- a ***y-x* diagram** (**McCabe-Thiele** diagram) (Figure 2.3)
- a ***Txy* diagram** (temperature-composition diagram) (Figure 2.4)
- an ***enthalpy-composition*** diagram

Note that, if the experiment is carried out in a *constant* temperature mode (where the pressure of the system is varied), a ***Pxy* diagram** is obtained (instead of a *Txy* diagram)

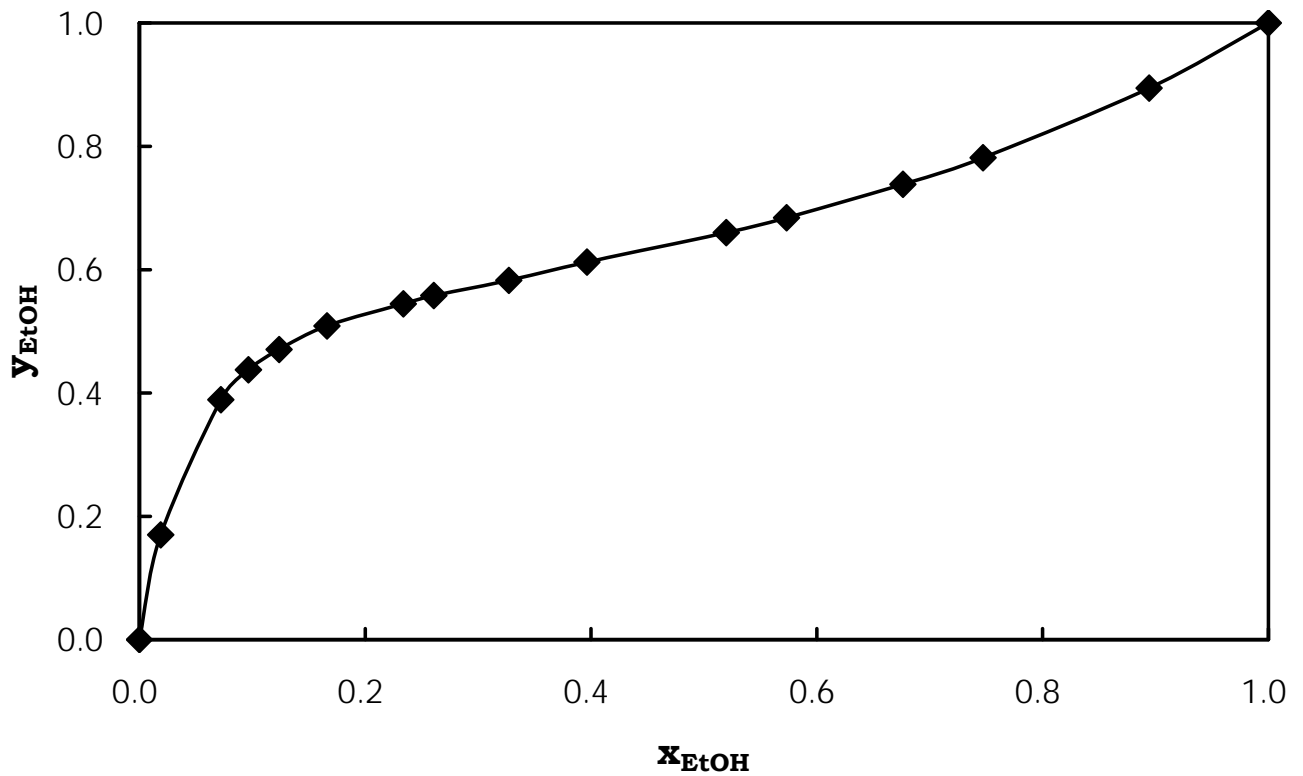


Figure 2.3: A $y-x$ diagram for the EtOH-water binary system
(A *McCabe-Thiele* diagram for the EtOH-water binary mixture)

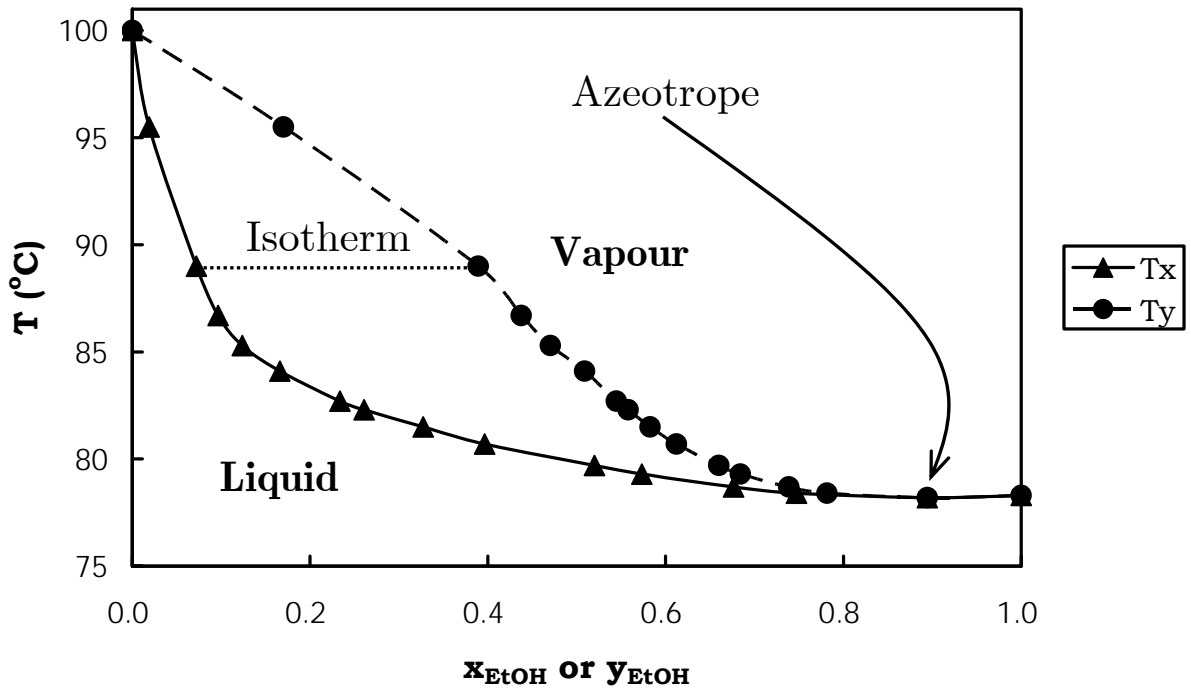


Figure 2.4: A Txy diagram for EtOH-water binary mixture

Note that, in Figure 2.4,

- a *solid* line ($T - x$) is a *saturated liquid* line
- a *dashed* line ($T - y$) is a *saturated vapour* line
- there is an azeotrope (???) in this system at the point where $x_{\text{EtOH}} = y_{\text{EtOH}} = 0.8943$

2.2 Binary Flash Distillation

Let's consider the flash distillation system (see Figure 2.1 on Page 3); the material balances of the system within the dashed boundary can be performed as follows

Overall balance

$$F = L + V \quad (2.1)$$

Species balance

$$z_i F = x_i L + y_i V \quad (2.2)$$

Re-arranging Eq. 2.2 for y_i gives

$$y_i = -\frac{L}{V} x_i + \frac{F}{V} z_i \quad (2.6)$$

Let's define

- $\frac{V}{F} \equiv f$: the *fraction* of the feed that *vaporises*
- $\frac{L}{F} \equiv q$: the *fraction* of the feed that *remains liquid*

Re-arranging Eq. 2.1 yields

$$L = F - V \quad (2.1a)$$

Thus, the term $\frac{L}{V}$ in Eq. 2.6 can be re-written, by combining with Eq. 2.1a, as

$$\frac{L}{V} = \frac{F - V}{V} = \frac{1 - \frac{V}{F}}{\frac{V}{F}}$$

$$\frac{L}{V} = \frac{1-f}{f} \quad (2.7)$$

Substituting Eq. 2.7 into Eq. 2.6:

$$y_i = -\frac{L}{V}x_i + \frac{F}{V}z_i \quad (2.6)$$

and noting that the term $\frac{F}{V}$ is, in fact, $\frac{1}{f}$ yields

$$y_i = -\frac{1-f}{f}x_i + \frac{z_i}{f} \quad (2.8)$$

Alternatively, re-arranging Eq. 2.1 yields

$$V = F - L \quad (2.1b)$$

The term $\frac{L}{V}$ in Eq. 2.6 can be also re-written as (this time, by combining with Eq. 2.1b)

$$\frac{L}{V} = \frac{L}{F-L} = \frac{\frac{L}{F}}{1-\frac{L}{F}}$$

$$\frac{L}{V} = \frac{q}{1-q} \quad (2.9)$$

Additionally, the term $\frac{F}{V}$ in Eq. 2.6 can be re-written as (once again, by combining with Eq. 2.1b)

$$\frac{F}{V} = \frac{F}{F-L} = \frac{1}{1-\frac{L}{F}}$$

$$\frac{F}{V} = \frac{1}{1-q} \quad (2.10)$$

Substituting Eqs. 2.9 & 2.10 into Eq. 2.6 results in

$$y_i = -\frac{q}{1-q} x_i + \left(\frac{1}{1-q} \right) z_i \quad (2.11)$$

Note that Eqs. 2.6, 2.8, and 2.11 are, in fact, *equivalent* to one another, and they are the “**operating equations**” for the flash tank, in which

- the *slopes* of Eqs. 2.6, 2.8, and 2.11 are

$$-\frac{L}{V}, \quad -\frac{1-f}{f}, \quad \text{and} \quad -\frac{q}{1-q}, \quad \text{respectively}$$

- the *Y-intercepts* of Eqs. 2.6, 2.8, and

$$2.11 \text{ are } \frac{F}{V} z_i, \quad \frac{z_i}{f}, \quad \text{and} \quad \left(\frac{1}{1-q} \right) z_i, \text{ respect-}$$

ively

The intersection of the equilibrium curve [see the y - x diagram (Figure 2.3) on Page 13] and the operating line is the solution (answer) of the material balances (this plot is called “**McCabe-Thiele diagram**”) for the flash distillation, as the *intersection* of the *equilibrium line* (curve) and the *operating line* is *the point* where the *system* (*i.e.* the flash tank) *reaches* the *equilibrium*

Note also that when $y_i = x_i$ (or $x_i = y_i$),

Eq. 2.6:

$$y_i = -\frac{L}{V}x_i + \frac{F}{V}z_i \quad (2.6)$$

becomes

$$y_i = -\frac{L}{V}y_i + \frac{F}{V}z_i$$

which can be re-arranged to

$$\left(1 + \frac{L}{V}\right)y_i = \frac{F}{V}z_i$$

$$\left(\frac{V + L}{V}\right)y_i = \frac{F}{V}z_i \quad (2.12)$$

However, since, from Eq. 2.1, $F = L + V$,
Eq. 2.12 can thus be re-written as

$$\frac{F}{V}y_i = \frac{F}{V}z_i \quad (2.13)$$

Therefore, $x_i = y_i = z_i$

This means (or implies) that the *intersection*
of the *operating line* and the $y_i = x_i$ *line* is, in
fact, the ***feed composition***

Consider the McCabe-Thiele diagram of the EtOH-water system for the case where $\frac{V}{F} = f = \frac{2}{3}$ and $z_{\text{EtOH}} = 0.40$

The *slope* of the operating line is $-\frac{1-f}{f} = -\frac{1-\frac{2}{3}}{\frac{2}{3}} = -\frac{1}{2}$, and the *Y-intercept* is $\frac{z_i}{f} = \frac{0.40}{\frac{2}{3}} = 0.60$

Thus, the solution to this case is as illustrated in Figure 2.5

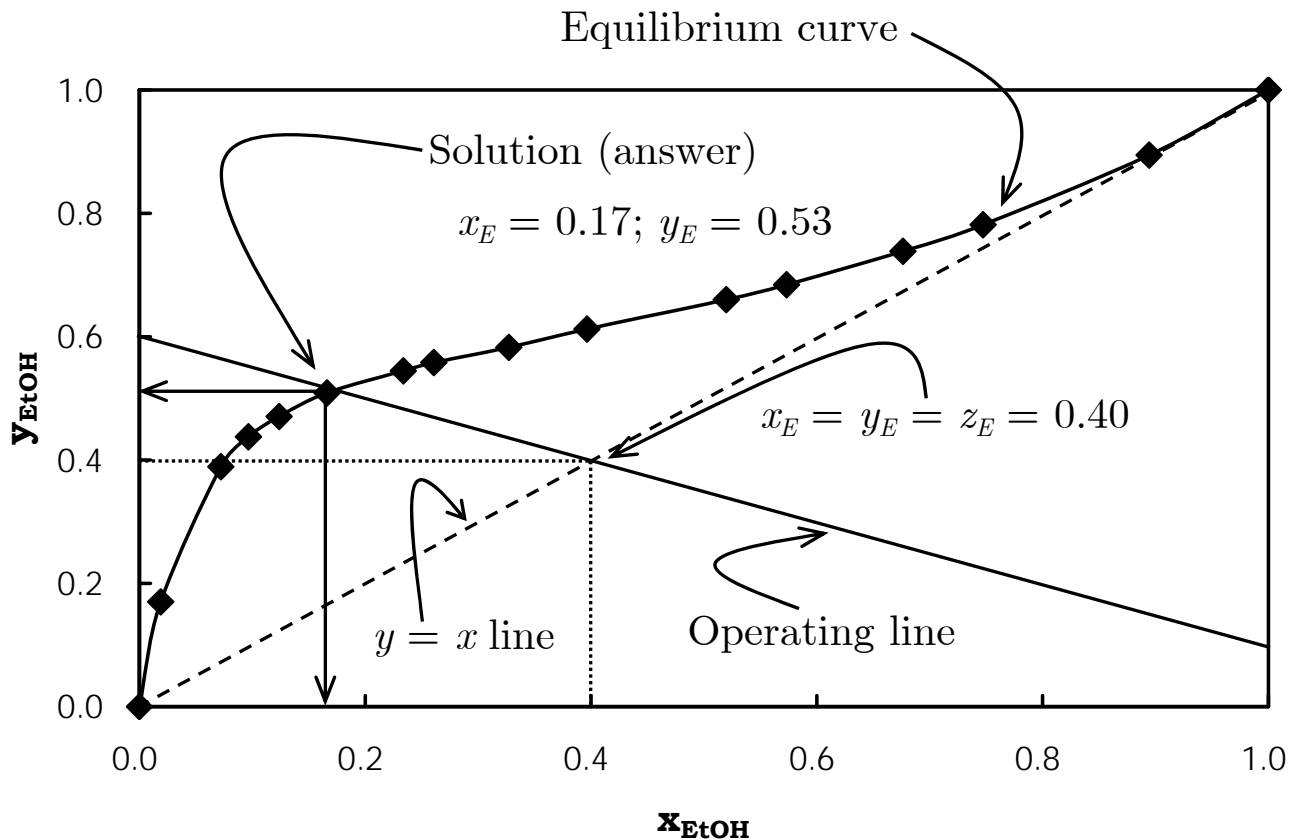


Figure 2.5: The graphical solution for a flash distillation

Substituting Eq. 2.1a:

$$L = F - V \quad (2.1a)$$

into Eq. 2.2:

$$z_i F = x_i L + y_i V \quad (2.2)$$

and re-arranging the resulting equation gives

$$z_i F = x_i (F - V) + y_i V$$

$$\begin{aligned}
z_i F &= x_i F - x_i V + y_i V \\
z_i F - x_i F &= -x_i V + y_i V \\
F(z_i - x_i) &= V(y_i - x_i)
\end{aligned}$$

$$\frac{V}{F} = f = \frac{(z_i - x_i)}{(y_i - x_i)} \quad (2.14)$$

Performing a similar derivation (try doing it yourself) for $\frac{L}{F}$ results in

$$\frac{L}{F} = q = \frac{(z_i - y_i)}{(x_i - y_i)} \quad (2.15)$$

In the case that an *analytical* solution is desired (in stead of the *graphical* solution—as illustrated in Figure 2.5), an *equilibrium curve* must be translated into the form of *equation*

For *ideal* systems (*i.e.*, the *gas phase* behaves as it is an *ideal-gas* mixture, while the *liquid phase* can be considered as an *ideal liquid solution*), the *equilibrium data* between x_i and y_i can be written in the form of “***relative volatility***: α_{AB} ”, which is defined as

$$\alpha_{AB} = \frac{y_A / x_A}{y_B / x_B} \quad (2.16)$$

For a *binary* mixture, where

$$x_B = 1 - x_A$$

and

$$y_B = 1 - y_A$$

Eq. 2.16 becomes

$$\alpha_{AB} = \frac{y_A / x_A}{(1 - y_A) / (1 - x_A)} \quad (2.17a)$$

or

$$\alpha_{AB} = \frac{y_A (1 - x_A)}{x_A (1 - y_A)} \quad (2.17b)$$

Re-arranging a Raoult's law:

$$y_i P = x_i P_i^* \quad (2.18)$$

where

P = total pressure of the system

P_i^* = vapour pressure of species i

results in

$$\frac{y_i}{x_i} = \frac{P_i^*}{P} \quad (2.19)$$

Substituting Eq. 2.19 into Eq. 2.16 for species A and B yields

$$\alpha_{AB} = \frac{\frac{P_A^*}{P}}{\frac{P_B^*}{P}} = \frac{P_A^*}{P_B^*} \quad (2.20)$$

Eq. 2.20 implies that the value of α_{AB} can be computed from the vapour-pressure data of the components (*e.g.*, species A & B) of the system

Writing Eq. 2.17a for species i gives

$$\alpha = \frac{y_i / x_i}{(1 - y_i) / (1 - x_i)} \quad (2.17c)$$

(note that Eq. 2.18c is **valid** *only* for a *binary mixture*)

Re-arranging Eq. 2.18c for y_i yields

$$y_i = \frac{x_i \alpha}{\left[1 + (\alpha - 1) x_i\right]} \quad (2.21)$$

Eq. 2.21 is an **equilibrium-curve** equation

To obtain the *analytical* solution for the flash distillation, equate Eq. 2.21 with one of the *operating-line* equation (*i.e.* Eq. 2.6, 2.8, or 2.11)

For example, when equating Eq. 2.21 with Eq. 2.8:

$$y_i = -\frac{1-f}{f} x_i + \frac{z_i}{f} \quad (2.8)$$

it results in

$$\frac{x_i \alpha}{[1 + (\alpha - 1)x_i]} = -\frac{1-f}{f}x_i + \frac{z_i}{f} \quad (2.22)$$

Re-arranging Eq. 2.22 yields

$$\frac{(1-f)}{f}(\alpha-1)x^2 + \left[\alpha + \frac{(1-f)}{f} - \frac{(\alpha-1)z}{f} \right]x - \frac{z}{f} = 0 \quad (2.23)$$

The answer (solution) of **Eq. 2.23** is the *analytical* solution of the **flash distillation** for a *binary* mixture

2.3 Multi-component VLE

From the ChE Thermodynamics II course, for the system with *more than 2 components*, the equilibrium data can, *more conveniently*, be presented in the form of the following equation (proposed by C.L. DePrieter in 1953):

$$y_i = K_i x_i \quad (2.24)$$

For many systems, it is safe—with an acceptable error—to assume that

$$K_i = K_i(T, P)$$

For light hydrocarbons, the value of K_i of each species can be obtained from the graph (called the “**K chart**” – Figures 2.6 and 2.7) prepared by DePriester when the temperature and pressure of the system are specified

Note that each plot/graph of each hydrocarbons can be written in the form of equation as follows

$$\ln K = \frac{a_{T_1}}{T^2} + \frac{a_{T_2}}{T} + a_{T_6} + a_{P_1} \ln P + \frac{a_{P_2}}{P^2} + \frac{a_{P_3}}{P} \quad (2.25)$$

in which the values of a_{T_1} , a_{T_2} , a_{T_6} , a_{P_1} , a_{P_2} , and a_{P_3} vary from substance to substance, and the units of T and P in Eq. 2.25 are °R and psia, respectively

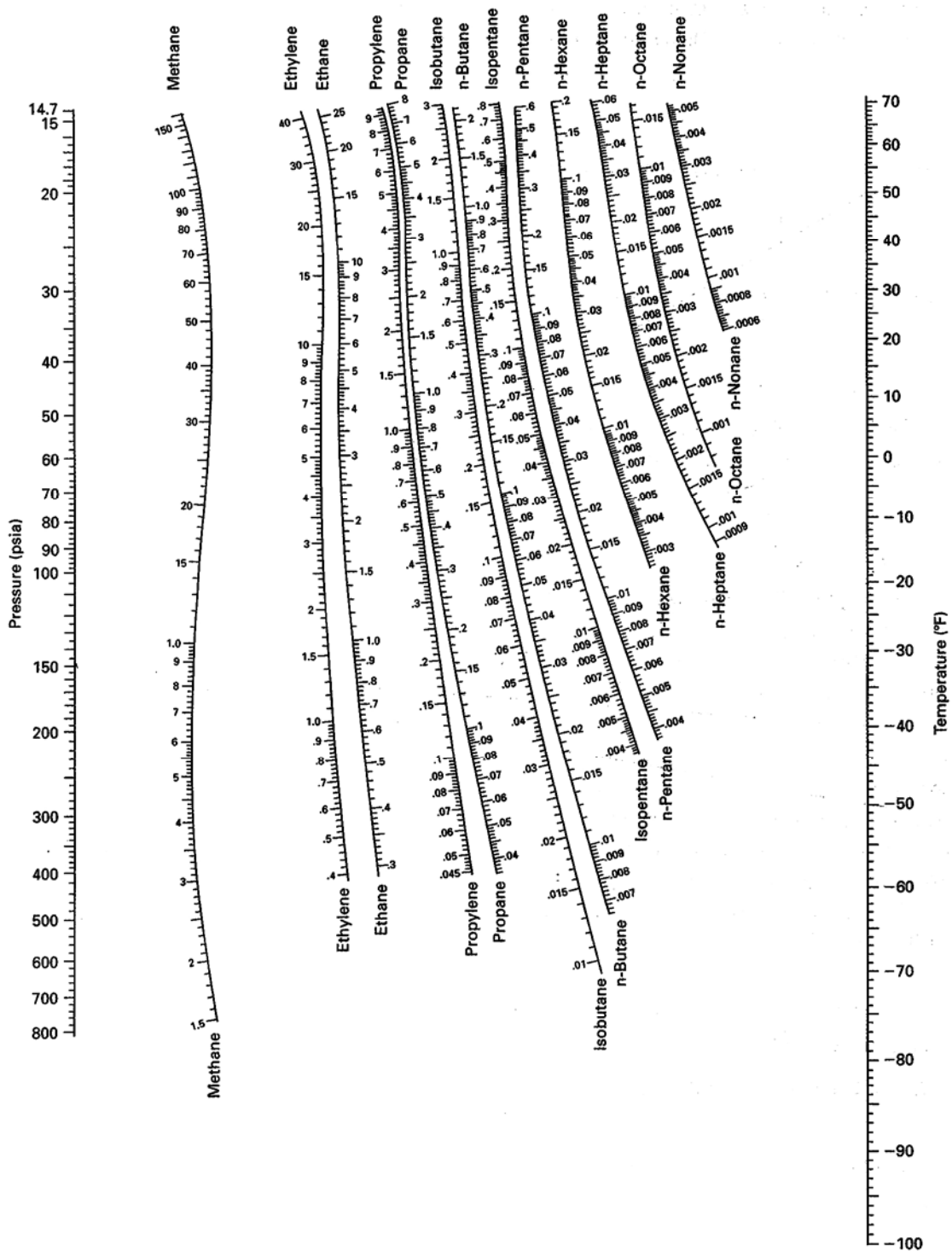


Figure 2.6: The K chart (low temperature range)

[from Introduction to Chemical Engineering Thermodynamics (7th ed)
by J.M. Smith, H.C. Van Ness, and M.M. Abbott]

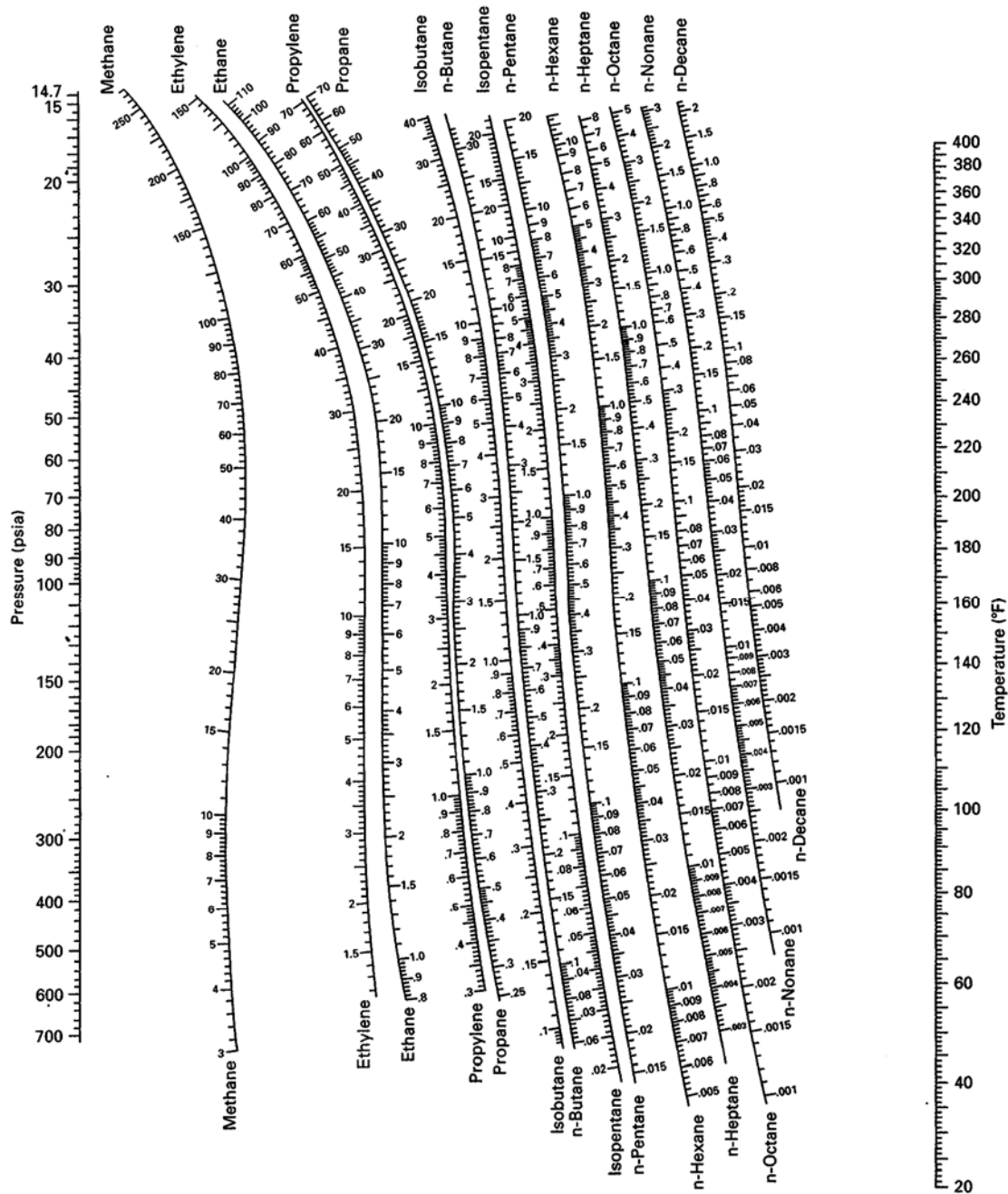


Figure 2.7: The K chart (high temperature range)

[from Introduction to Chemical Engineering Thermodynamics (7th ed)
by J.M. Smith, H.C. Van Ness, and M.M. Abbott]

The meaning of K_i on the K chart can be described *mathematically* by the *original* Raoult's law and the *modified* Raoult's law as follows

Re-arranging 2.24:

$$y_i = K_i x_i \quad (2.24)$$

results in

$$\frac{y_i}{x_i} = K_i \quad (2.26)$$

Equating Eq. 2.26 with Eq. 2.19:

$$\frac{y_i}{x_i} = \frac{P_i^*}{P} \quad (2.19)$$

yields

$$K_i = \frac{P_i^*}{P} \quad (2.27)$$

In the case of *non-ideal* systems, Raoult's law is modified to

$$y_i P = x_i \gamma_i P_i^* \quad (2.28)$$

where γ_i is an activity coefficient of species i , which can be calculated using, *e.g.*, Margules or Van Laar equations

Re-arranging Eq. 2.28 gives

$$\frac{y_i}{x_i} = \frac{\gamma_i P_i^*}{P} \quad (2.29)$$

Once again, equating Eq. 2.29 with Eq. 2.26 results in

$$K_i = \frac{\gamma_i P_i^*}{P} \quad (2.30)$$

2.4 Multi-component Flash Distillation

Let's start with Eq. 2.2:

$$z_i F = x_i L + y_i V \quad (2.2)$$

which is a *species-balance* equation for the flash distillation

Substituting Eq. 2.24:

$$y_i = K_i x_i \quad (2.24)$$

into Eq. 2.2 results in

$$z_i F = x_i L + K_i x_i V \quad (2.31)$$

Writing L in Eq. 2.31 as $F - V$ (see Eq. 2.1a on Page 16) yields

$$z_i F = x_i (F - V) + K_i x_i V \quad (2.32)$$

Re-arranging Eq. 2.32 for x_i gives

$$x_i = \frac{z_i F}{F + (K_i - 1)V} \quad (2.33)$$

Dividing numerator (เศษ) and denominator (ส่วน) of the right hand side (RHS) of Eq. 2.33 by F results in

$$x_i = \frac{z_i}{1 + (K_i - 1)\frac{V}{F}} \quad (2.34)$$

Re-arranging Eq. 2.24:

$$y_i = K_i x_i \quad (2.24)$$

once again gives

$$x_i = \frac{y_i}{K_i} \quad (2.35)$$

Substituting Eq. 2.35 into Eq. 2.34 and rearranging the resulting equation yields

$$\frac{y_i}{K_i} = \frac{z_i}{1 + (K_i - 1)\frac{V}{F}}$$

$$y_i = \frac{z_i K_i}{1 + (K_i - 1)\frac{V}{F}} \quad (2.36)$$

Since it is required that, at equilibrium, $\sum x_i = 1$ and $\sum y_i = 1$, we obtain the following relationships (by tanking summation to Eqs. 2.34 and 2.36, respectively):

$$\sum \left(\frac{z_i}{1 + (K_i - 1) \frac{V}{F}} \right) = 1 \quad (2.37)$$

and

$$\sum \left(\frac{z_i K_i}{1 + (K_i - 1) \frac{V}{F}} \right) = 1 \quad (2.38)$$

To solve for the solution for any *multi*-component (more than 2 components) system, $\frac{V}{F}$ is varied, using a *trial & error* technique, until both Eqs. 2.37 & 2.38 are satisfied

Unfortunately, however, since these are *non-linear* equations, they **do not have good convergence** properties

Hence, if the first guess of $\frac{V}{F}$ is not good enough (*i.e.* **too far from** the *real* answer), the correct solution may not be obtained

To enhance the efficiency of the trial & error process, the following technique is suggested

Since both $\sum x_i$ and $\sum y_i$ are equal to unity (1), subtracting Eq. 2.37 from Eq. 2.38 gives

$$\sum \left(\frac{z_i K_i}{1 + (K_i - 1) \frac{V}{F}} \right) - \sum \left(\frac{z_i}{1 + (K_i - 1) \frac{V}{F}} \right) = 0 \quad (2.39)$$

Let's define the left hand side (LHS) of Eq.

2.39 as

$$g = \sum \left(\frac{z_i K_i}{1 + (K_i - 1) \frac{V}{F}} \right) - \sum \left(\frac{z_i}{1 + (K_i - 1) \frac{V}{F}} \right)$$

which can be re-arranged to

$$g = \sum \left(\frac{(K_i - 1) z_i}{1 + (K_i - 1) \frac{V}{F}} \right) \quad (2.40)$$

Note that g is a function of $\frac{V}{F}$ or

$$g = g \left(\frac{V}{F} \right)$$

To solve for the solution, it is required that
that

$$g = 0$$

We can employ a numerical method, such as a “*Newtonian convergence procedure*” to solve for the solution as follows

Let’s define the value of g for trial k as g_k and the value of g for the trial $k + 1$ as g_{k+1}

The equation for the *Newtonian convergence* procedure is

$$g_{k+1} - g_k = \frac{dg_k}{d\left(\frac{V}{F}\right)} \Delta\left(\frac{V}{F}\right) \quad (2.41)$$

Note that $\frac{dg_k}{d\left(\frac{V}{F}\right)}$ is the value of the derivative

of the function for trial k

Re-arranging Eq. 2.41 yields

$$\Delta\left(\frac{V}{F}\right) = \frac{g_{k+1} - g_k}{\frac{dg_k}{d\left(\frac{V}{F}\right)}} \quad (2.42)$$

As the *ultimate* goal is to have the value of $g_{k+1} = 0$, Eq. 2.42 becomes

$$\Delta\left(\frac{V}{F}\right) = \frac{0 - g_k}{\frac{dg_k}{d\left(\frac{V}{F}\right)}}$$

$$\Delta\left(\frac{V}{F}\right) = \frac{-g_k}{\frac{dg_k}{d(V / F)}} \quad (2.43)$$

Since

$$\Delta \left(\frac{V}{F} \right) = \left(\frac{V}{F} \right)_{k+1} - \left(\frac{V}{F} \right)_k$$

Eq. 2.43 can be re-written as

$$\Delta \left(\frac{V}{F} \right) = \left(\frac{V}{F} \right)_{k+1} - \left(\frac{V}{F} \right)_k = \frac{-g_k}{\left[\frac{dg_k}{d(V/F)} \right]} \quad (2.44)$$

By employing Eq. 2.40, the term $\frac{dg_k}{d(V/F)}$

in Eq. 2.44 can be derived as

$$\frac{dg_k}{d \left(\frac{V}{F} \right)} = - \sum \frac{(K_i - 1)^2 z_i}{\left[1 + (K_i - 1) \frac{V}{F} \right]^2} \quad (2.45)$$

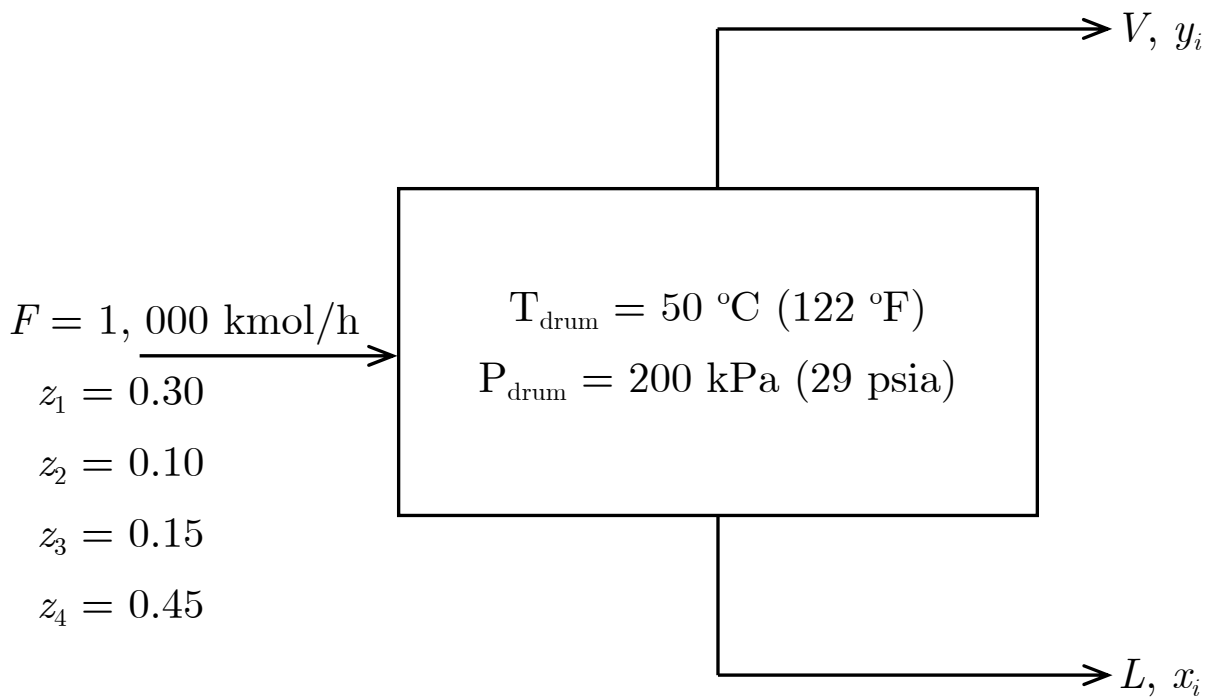
Hence, the next guess of $\frac{V}{F}$, which may enable $g_{k+1} = 0$, and, thus, makes $\sum x_i = 1$ and $\sum y_i = 1$ can be obtained from the following equation:

$$\left(\frac{V}{F}\right)_{k+1} = \left(\frac{V}{F}\right)_k - \frac{g_k}{\left[\frac{dg_k}{d(V/F)}\right]} \quad (2.46)$$

or

$$\left(\frac{V}{F}\right)_{k+1} = \left(\frac{V}{F}\right)_k + \frac{\sum \left(\frac{(K_i - 1)z_i}{1 + (K_i - 1)\frac{V}{F}} \right)}{\sum \frac{(K_i - 1)^2 z_i}{\left[1 + (K_i - 1)\frac{V}{F}\right]^2}} \quad (2.47)$$

Example A flash chamber operating at 50 °C (122 °F) and 200 kPa (29 psia) is separating 1,000 kmol/h of feed containing 30 mol% propane, 10% *n*-butane, and 15% *n*-pentane, and 45% *n*-hexane. Find the product compositions and flow rates



Note that, 1, 2, 3, & 4 = propane, *n*-butane, *n*-pentane, & *n*-hexane, respectively

At $T = 50\text{ }^{\circ}\text{C}$ ($122\text{ }^{\circ}\text{F}$) and $P = 200\text{ kPa}$ (29 psia), the value of K_i read from the K chart of each species is as follows

- $K_1 = 7.0$
- $K_2 = 2.4$
- $K_3 = 0.80$
- $K_4 = 0.30$

Let's start with $\frac{V}{F} = 0.1$, and the value of

$$g\left(\frac{V}{F}\right) = \sum \left[\frac{(K_i - 1)z_i}{1 + (K_i - 1)\frac{V}{F}} \right] \text{ can be calculated as}$$

follows

$$g(0.1) = \frac{(7.0 - 1)(0.30)}{1 + (7.0 - 1)(0.1)} + \frac{(2.4 - 1)(0.10)}{1 + (2.4 - 1)(0.1)}$$

$$+ \frac{(0.80 - 1)(0.15)}{1 + (0.80 - 1)(0.1)} + \frac{(0.30 - 1)(0.45)}{1 + (0.30 - 1)(0.1)}$$

$$g(0.1) = 0.88$$

which is **NOT** equal to **zero (0)** yet

Employing Eq. 2.45 to calculate the value of

$$\frac{dg_k}{d\left(\frac{V}{F}\right)} = - \sum \frac{(K_i - 1)^2 z_i}{\left[1 + (K_i - 1)\frac{V}{F}\right]^2} \text{ yields}$$

$$\frac{dg_k}{d\left(\frac{V}{F}\right)} = - \left\{ \frac{(7.0 - 1)^2 (0.30)}{\left[1 + (7.0 - 1)(0.1)\right]^2} + \frac{(2.4 - 1)^2 (0.10)}{\left[1 + (2.4 - 1)(0.1)\right]^2} \right.$$

$$\left. + \frac{(0.80 - 1)^2 (0.15)}{\left[1 + (0.80 - 1)(0.1)\right]^2} + \frac{(0.30 - 1)^2 (0.45)}{\left[1 + (0.30 - 1)(0.1)\right]^2} \right\}$$

$$\frac{dg_k}{d\left(\frac{V}{F}\right)} = -4.63$$

Then, using Eq. 2.46 (or Eq. 2.47) to compute the value of the next guess of $\frac{V}{F}$ gives

$$\left(\frac{V}{F}\right)_{k+1} = \left(\frac{V}{F}\right)_k - \frac{g_k}{\left[\frac{dg_k}{d(V/F)}\right]}$$

$$\left(\frac{V}{F}\right)_{k+1} = (0.1) - \frac{0.88}{(-4.63)}$$

$$\left(\frac{V}{F}\right)_{k+1} = 0.29$$

Then, repeat the process all over again, until we obtain the value of $\frac{V}{F}$ that makes $g = 0$

The corresponding value of $\frac{V}{F}$ that makes $g = 0$ for this Example is found to be **0.51**

After obtaining the correct value of $\frac{V}{F}$, the values of x_i and y_i of each species can be calculated as follows

The value of x_i can be calculated from Eq. 2.34, as can be illustrated for propane (C_3H_8 – species 1) as follows

$$\begin{aligned}
 x_1 &= \frac{z_1}{1 + (K_1 - 1)\frac{V}{F}} \\
 &= \frac{(0.30)}{1 + (7.0 - 1)(0.51)} \\
 x_1 &= 0.074
 \end{aligned}$$

Then, the value of y_i can be computed using Eq. 2.24:

$$y_i = K_i x_i \quad (2.24)$$

For propane (species 1),

$$y_1 = (7.0)(0.074) = 0.518$$

Performing the same calculations for other species results in

$$x_2 = 0.058 \quad y_2 = 0.140$$

$$x_3 = 0.167 \quad y_3 = 0.134$$

$$x_4 = 0.700 \quad y_4 = 0.210$$

Since $\frac{V}{F} = 0.51$ and $F = 1,000$ kmol/h,

$V = 510$ kmol/h, and $L = 490$ kmol/h

Thus, the flow rates of each species in the *liquid* and *gas* phases can be computed as follows

Liquid phase ($l_i = x_i L$):

- Propane: $(0.074)(490) = 36.26$ kmol
- *n*-butane: $(0.058)(490) = 28.42$ kmol
- *n*-pentane: $(0.167)(490) = 81.83$ kmol
- *n*-hexane: $(0.700)(490) = 343.0$ kmol
- **TOTAL** = **489.5** kmol

Gas phase ($v_i = y_i V$):

- Propane: $(0.518)(510) = 264.2$ kmol
- *n*-butane: $(0.140)(510) = 71.40$ kmol
- *n*-pentane: $(0.134)(510) = 68.34$ kmol
- *n*-hexane: $(0.210)(510) = 107.1$ kmol
- **TOTAL** = **511.0** kmol

Another approach to solve this Example is as already studied from ChE Thermodynamics II; the details are as follows

Substituting Eq. 2.24:

$$y_i = K_i x_i \quad (2.24)$$

into the species balance equation (Eq. 2.2):

$$z_i F = x_i L + y_i V \quad (2.2)$$

and re-arranging the resulting equation gives

$$\begin{aligned} z_i F &= x_i L + K_i x_i V \\ &= x_i \left(L + K_i V \right) \\ z_i F &= x_i L \left(1 + K_i \frac{V}{L} \right) \end{aligned}$$

$$x_i L = \frac{z_i F}{\left(1 + K_i \frac{V}{L} \right)} \quad (2.48)$$

For the feed to become liquid, $\sum x_i = 1$

Thus,

$$\sum x_i L = L \sum x_i = L(1) = L = \sum \frac{z_i F}{\left(1 + K_i \frac{V}{L}\right)} \quad (2.49)$$

Substituting Eq. 2.35:

$$x_i = \frac{y_i}{K_i} \quad (2.35)$$

into Eq. 2.2 and re-arranging the resulting equation yields

$$\begin{aligned} z_i F &= \frac{y_i}{K_i} L + y_i V \\ &= \frac{y_i L + y_i K_i V}{K_i} \end{aligned}$$

$$\begin{aligned}
z_i K_i F &= y_i L + y_i K_i V \\
&= y_i (L + K_i V) \\
z_i K_i F &= y_i V \left(\frac{L}{V} + K_i \right)
\end{aligned}$$

$$y_i V = \frac{z_i K_i F}{\left(\frac{L}{V} + K_i \right)} \quad (2.50)$$

For the feed to become vapour, $\sum y_i = 1$

Hence,

$$\sum y_i V = V \sum y_i = V (1) = V = \sum \frac{z_i K_i F}{\left(\frac{L}{V} + K_i \right)} \quad (2.51)$$

To solve for the value of L , the trial & error technique must be employed such that the value of L is guessed, and the corresponding value of V is obtained from the fact that $V = F - L$

Then, the value of L is calculated using Eq. 2.49

The trial & error process is iterated (ทำซ้ำ ๆ กัน) until the guessed value of L is equal to the value of L computed from Eq. 2.49

Likewise, to obtain the value of V , the value of V is guessed, and the corresponding value of L is computed from the fact that $L = F - V$

The value of the guessed V and the corresponding value of L are then used to calculate the value of V using Eq. 2.51

The iteration of the trial & error is performed until the guessed value of V is equal to the calculated value of V using Eq. 2.51

In this Example, both values of V and L must firstly be determined; thus, we can make a guess for either L or V

Let's start with the **first guess** of L as **100 kmol**; hence, the corresponding value of V is

$$V = F - L = 1,000 - 100 = 900 \text{ kmol}$$

The value of L can then be computed using Eq. 2.49 as illustrated in the following Table:

Species	z_i	K_i	$l_i = \frac{z_i F}{\left(1 + K_i \frac{V}{L}\right)}$
Propane	0.30	7.0	$\frac{(0.30)(1,000)}{\left[1 + (7.0)\left(\frac{900}{100}\right)\right]} = 4.7$
<i>n</i> -Butane	0.10	2.4	4.4
<i>n</i> -Pentane	0.15	0.80	18.3
<i>n</i> -Hexane	0.45	0.30	121.6
$\Sigma =$	1.00	$L =$	149.0

The guessed value of L is NOT equal to the value of L calculated using Eq. 2.49; thus, a new guess is needed

The iteration is performed until the guessed value of L is equal to the value of L computed using Eq. 2.49, and the *resulting* value of L is found to be **488.6 kmol** (and the corresponding value of V is $1,000 - 488.6 = 511.4$ kmol), which yields

Species	z_i	K_i	$l_i = \frac{z_i F}{\left(1 + K_i \frac{V}{L}\right)}$
Propane	0.30	7.0	$\frac{(0.30)(1,000)}{\left[1 + (7.0)\left(\frac{511.4}{488.6}\right)\right]} = 36.0$
<i>n</i> -Butane	0.10	2.4	28.5
<i>n</i> -Pentane	0.15	0.80	81.6
<i>n</i> -Hexane	0.45	0.30	342.5
$\Sigma =$	1.00	$L =$	488.6

The composition of each species in each phase can, thus, be calculated as follows

Species	z_i	$f_i = z_i F$	l_i	$x_i = \frac{l_i}{L}$
Propane	0.30	300	36.0	$\frac{36.0}{488.6} = 0.074$
<i>n</i> -Butane	0.10	100	28.5	0.058
<i>n</i> -Pentane	0.15	150	81.6	0.167
<i>n</i> -Hexane	0.45	450	342.5	0.701
$\Sigma =$	1.00	1,000	488.6	1.001

Species	$f_i = z_i F$	l_i	$v_i = f_i - l_i$	$y_i = \frac{v_i}{V}$
Propane	300	36.0	$300 - 36.0 = 264.0$	$\frac{264.0}{511.4} = 0.516$
<i>n</i> -Butane	100	28.5	71.5	0.140
<i>n</i> -Pentane	150	81.6	68.4	0.134
<i>n</i> -Hexane	450	342.5	107.5	0.210
$\Sigma =$	1,000	488.6	511.4	1.000