Chapter 5: Introduction to Multi-component Distillation

Normally, for any *distillation problems*, there are

$$\boldsymbol{C + 6}$$

degree of freedoms, where $\boldsymbol{C}$ is the number of components

For example, for a *binary mixture* distillation problem, the *degree of freedom* is

$$\boldsymbol{2} + 6 = \mathbf{8}$$

In the *design* problem for a *binary* mixture, the following **8** *variables* are usually *specified*:

- Feed flow rate $\left(F\right)$
- Feed composition $\left(z_i\right)$

  (note that, normally, $i =$ a *more volatile* component: MVC)
- Feed quality $\left(q\right)$
- Distillate composition $\left(x_D\right)$
- Bottom composition $\left(x_B\right)$
- Distillate temperature/enthalpy (*e.g.*, distillate is a saturated liquid)
- External reflux ratio $\left(\frac{L_o}{D}\right)$
- Optimal feed stage

Since the ***number*** of ***specified*** **variables** (**8**) is ***equal*** to that of the **degrees of freedom** (**8**), the problem can be solved, which means that we can

- *draw* all *operating* lines and the *feed* line(s)
- *step off stages* – to *find* the *number* of *equilibrium stages* required for that problem

For a ***ternary*** **(3-component)** mixture, the degree of freedom is

$$\boldsymbol{3} + 6 = \mathbf{9}$$

Thus, we need to have **9** *specified variables* to *solve* the *problem*

The common *specified* variables for a *ternary mixture* problem include the following:

- Feed flow rate $\left(F\right)$
- Feed composition $\left(z_i\right)$ for 2 components (at least) (*e.g.*, z_1 and z_2)
- Feed quality/enthalpy/temperature (q or h_F or T_F)
- Distillate composition (*e.g.*, $x_{1,\text{ dist}}$, D, **fractional recovery of *at least* one component: $\boldsymbol{FR_{D_i}}$**)
- Bottom composition (*e.g.*, $x_{2,\text{ bot}}$, B, **fractional recovery of *at least* one component: $\boldsymbol{FR_{B_i}}$**)
- External reflux $\left(\dfrac{L}{D}\right)$ or boil-up $\left(\dfrac{\bar{V}}{B}\right)$ ratio or heating load $\left(Q_R\right)$

- Reflux temperature/enthalpy (*e.g.*, T_{reflux}, saturated liquid reflux)
- Optimal feed stage

What is **"fractional recovery"** $\left(\boldsymbol{FR}\right)$?

Let's consider the following Example

Example The *ternary mixture* feed contains 30 mol% ethane (C_2), 40% propane (C_3), and the remaining *n*-butane (C_4)

If we want to obtain **99% recovery** of $\mathbf{C_3}$ in the **distillate**, write the equation expressing the relationship between the amount of C_3 in the *feed* and that in the *distillate*

The number of **moles** of $\mathbf{C_3}$ in the **feed** is

$$\left[C_3\right]_{\text{feed}} = z_{C_3} F \qquad (5.1)$$

The number of **moles** of $\mathbf{C_3}$ in the **distillate** is

$$\left[C_3\right]_{\text{dist}} = x_{D_{C_3}} D \qquad (5.2)$$

The number of **moles** of $\mathbf{C_3}$ in the **bottom** is

$$\left[C_3\right]_{\text{bottom}} = x_{B_{C_3}} B \qquad (5.3)$$

The number of **moles** of $\mathbf{C_3}$ in the **distillate** *combined* with the number of **moles** of $\mathbf{C_3}$ in the **bottom**:

$$\left[C_3\right]_{\text{dist}} + \left[C_3\right]_{\text{bottom}}$$

is, of course,

$$\left[C_3\right]_{\text{feed}} = z_{C_3} F$$

Thus, we can write the following equations:

$$\left[\mathrm{C}_3\right]_{\text{feed}} = \left[\mathrm{C}_3\right]_{\text{dist}} + \left[\mathrm{C}_3\right]_{\text{bottom}} \tag{5.4a}$$

and

$$z_{\mathrm{C}_3} F = x_{D_{\mathrm{C}_3}} D + x_{B_{\mathrm{C}_3}} B \tag{5.4b}$$

Dividing Eq. 5.4b with $z_{\mathrm{C}_3} F$ gives

$$1 = \frac{x_{D_{\mathrm{C}_3}} D}{z_{\mathrm{C}_3} F} + \frac{x_{B_{\mathrm{C}_3}} B}{z_{\mathrm{C}_3} F} \tag{5.5}$$

The term $\boldsymbol{\frac{x_{D_{C_3}} D}{z_{C_3} F}}$ in Eq. 5.5 is the **portion** of **$\mathbf{C_3}$** in the **feed** that **goes out** in the **distillate**

Likewise, the term $\boldsymbol{\frac{x_{B_{C_3}} B}{z_{C_3} F}}$ is the **portion** of **$\mathbf{C_3}$** that **comes out** in the **bottom**

The term $\dfrac{\boldsymbol{x_{D_{\mathrm{C_3}}} D}}{\boldsymbol{z_{C_3} F}}$ is called the **fractional recovery of $\mathbf{C_3}$ in the distillate** $\left(\boldsymbol{FR_{\mathrm{C_3}}}\right)_{\mathbf{dist}}$, while the term $\dfrac{\boldsymbol{x_{B_{\mathrm{C_3}}} B}}{\boldsymbol{z_{C_3} F}}$ is called the **fractional recovery of $\mathbf{C_3}$ in the bottom** $\left(\boldsymbol{FR_{\mathrm{C_3}}}\right)_{\mathbf{bottom}}$

Thus, the **relationship** between the amount of $\mathbf{C_3}$ in the **feed** and that in the **distillate** can be written as follows

$$\left(FR_{\mathrm{C_3}}\right)_{\mathrm{dist}} = \frac{x_{D_{\mathrm{C_3}}} D}{z_{\mathrm{C_3}} F}$$

$$x_{D_{\mathrm{C_3}}} D = \left(FR_{\mathrm{C_3}}\right)_{\mathrm{dist}} z_{\mathrm{C_3}} F \tag{5.6}$$

Likewise, the **relationship** between $\mathbf{C_3}$ in the **feed** and that in the **bottom** can be written as follows

$$\left(FR_{\mathrm{C}_3}\right)_{\text{bottom}} = \frac{x_{B_{\mathrm{C}_3}} B}{z_{\mathrm{C}_3} F}$$

$$x_{B_{\mathrm{C}_3}} B = \left(FR_{\mathrm{C}_3}\right)_{\text{bottom}} z_{\mathrm{C}_3} F \qquad (5.7)$$

Eq. 5.5:

$$1 = \frac{x_{D_{\mathrm{C}_3}} D}{z_{\mathrm{C}_3} F} + \frac{x_{B_{\mathrm{C}_3}} B}{z_{\mathrm{C}_3} F} \qquad (5.5)$$

can also be written in another form as follows

$$1 = \left(FR_{\mathrm{C}_3}\right)_{\text{dist}} + \left(FR_{\mathrm{C}_3}\right)_{\text{bottom}} \qquad (5.8)$$

which can be re-arrange to

$$\left(FR_{\mathrm{C}_3}\right)_{\text{bottom}} = 1 - \left(FR_{\mathrm{C}_3}\right)_{\text{dist}} \qquad (5.9a)$$

or

$$\left(FR_{\mathrm{C}_3}\right)_{\mathrm{dist}} = 1 - \left(FR_{\mathrm{C}_3}\right)_{\mathrm{bottom}} \qquad (5.9\mathrm{b})$$

Hence, Eq. 5.7 can be written in another form, by combining with Eq. 5.9a, as follows

$$x_{B_{\mathrm{C}_3}} B = \left[1 - \left(FR_{\mathrm{C}_3}\right)_{\mathrm{dist}}\right] z_{\mathrm{C}_3} F \qquad (5.10)$$

Thus, in this Example, we can write the equation expressing the relationship between the amount of C_3 in the *feed* and that in the *distillate* as follows

$$x_{D_{\mathrm{C}_3}} D = \left(FR_{\mathrm{C}_3}\right)_{\mathrm{dist}} z_{\mathrm{C}_3} F$$

$$x_{D_{\mathrm{C}_3}} D = \left(0.99\right)\left(0.40\right) F = 0.396F$$

The equation expressing the relationship between the amount of C_3 in the *feed* and that in the *bottom* is

$$x_{B_{\mathrm{C}_3}} B = \left[1 - \left(FR_{\mathrm{C}_3}\right)_{\mathrm{dist}}\right] z_{\mathrm{C}_3} F$$

$$x_{B_{\mathrm{C}_3}} B = \left[1 - 0.99\right]\left(0.40\right) F = 0.004F$$

As described previously, we are allowed to have $\boldsymbol{C + 6}$ variables for the $\boldsymbol{C}$**-component** distillation problems

Accordingly, NOT all components' concentrations can be specified, and this makes the *multi*-component distillation problems different and **more difficult** than the *binary-mixture* problems

The components that have their *fractional recoveries* $\left(FR_i\right)$ **specified** = the ***key*** **components**

The **most volatile** (or the **lightest**) ***key*** component is called the **light key (LK)**

The **least volatile** (or the **heaviest**) ***key*** component is called **heavy key (HK)**

All other components are called the **non-keys** – or the **non-key components (NKs)**

Any **non-keys** that are **more volatile** (*i.e.* **lighter**) than the *light key* (LK) are called the ***light*** **non-keys (LNKs)**

On the contrary, any **non-keys** that are **less volatile** (*i.e.* **heavier**) than the *heavy key* (HK) are called the ***heavy*** **non-keys (HNKs)**

Consider the design distillation problem for the *multi-component* systems in Figure 5.1

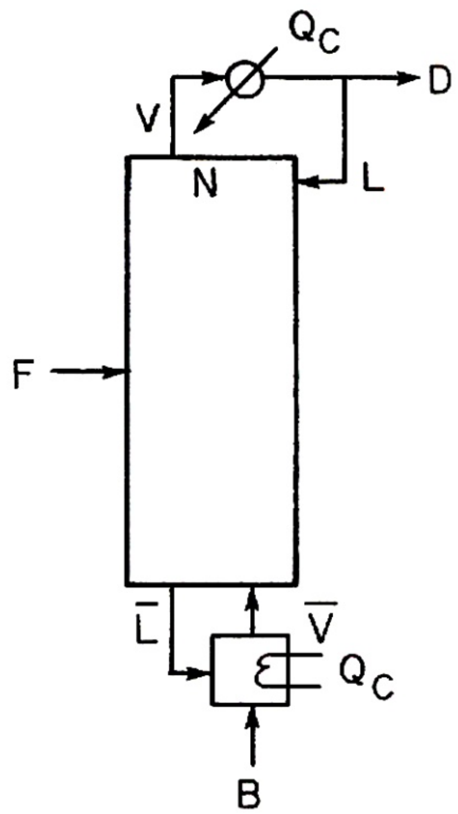


Figure 5.1: The distillation column for the multi-component system

(from "Separation Process Engineering" by Wankat, 2007)

Performing *material* and *energy* balances for this problem yields

Overall material balance

$$F = D + B \tag{5.11}$$

Species balance

$$z_i F = x_{i,\,\text{bot}} B + x_{i,\,\text{dist}} D \tag{5.12}$$

External energy balance

$$h_F F + Q_C + Q_R = h_B B + h_D D \tag{5.13}$$

Note that we can have *as high as* $\boldsymbol{C}$**–1** *independent* equations for Eq. 5.12 ($\boldsymbol{C}$ = number of components), because

$$\sum x_{i,\,\text{dist}} = 1 \tag{5.14a}$$

and

$$\sum x_{i,\,\text{bot}} = 1 \tag{5.14b}$$

For the **3-component** problems, the **unknowns** include

- ***B*** and ***D*** (2 unknowns)
- ***two*** out of $x_{1,\ \mathrm{dist}}$, $x_{2,\ \mathrm{dist}}$, and $x_{3,\ \mathrm{dist}}$ (2 unknowns)
- ***two*** out of $x_{1,\ \mathrm{bot}}$, $x_{2,\ \mathrm{bot}}$, and $x_{3,\ \mathrm{bot}}$ (2 unknowns)

In total, there are **6 unknowns** for this *3-component* distillation problem

By performing *only* **external** material balances (both *overall* and *species* balances), we can have *as high as*

- **1** *overall-balance* equation
- **2** *species-balance* equations
- **2** equations from Eq. **5.14a** and **5.14b**

which adds up to **5** *independent* equations – still ***NOT enough*** (as we **need 6** equations)

To obtain another *additional* equation, we can perform either

- *external* **energy** balance (*i.e.* Eq. 5.13)

or

- a *stage-by-stage* **internal** balance

Unfortunately, however, by **adding *such* equations**, it will **create *another* unknown(s)**; thus, this is **NOT** a **good choice**

To solve this kind of problem, we have to employ the ***trial & error*** technique, by carrying out the following procedure:

1) Make a **guess** for the number of **moles** (or **mole fraction**) of **one** *unknown* component in the *distillate* or the *bottom*
2) **Solve** the **problem** (by using that *guessed* variable)
3) Finally, **check** if **all equations** (especially Eqs. **5.14a** and **5.14b**) are ***true***

To enable us to **make** an ***excellent*** **first guess**, it is recommended that we *firstly* assume that

- all *light* non-keys (LNKs) appear *only* in the *distillate*, or

$$x_{\text{LNK, bot}} = 0 \tag{5.15}$$

and

- all *heavy* non-keys (HNKs) appear *only* in the *bottom*, or

$$x_{\text{HNK, dist}} = 0 \tag{5.16}$$

The Example on the next Page illustrates how to solve the *multi-component* distillation problem using the *trial & error* technique and the *principles* of *light* non-keys (LNKs) and *heavy* non-keys (HNKs)

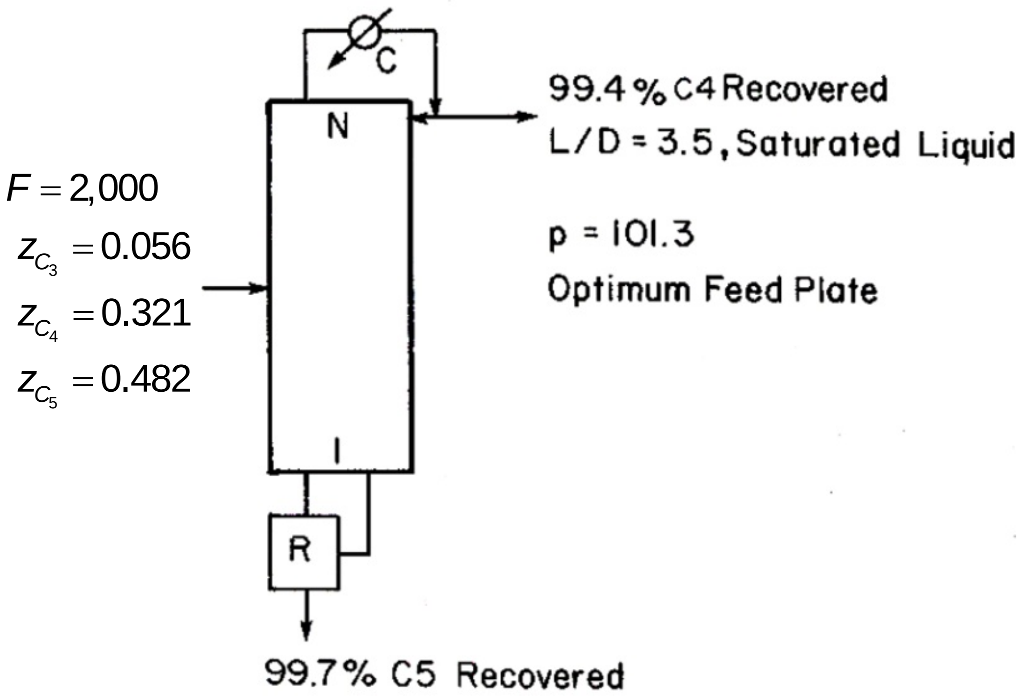
Example The 2,000 kmol/h *saturated liquid* feed with the composition of **0.056** *mole fraction* of **propane**, **0.321 *n*-butane**, **0.482 *n*-pentane**, and the *remaining* ***n*-hexane** is to be distilled in an *atmospheric* distillation column

The column has a *total* condenser and a *partial* re-boiler, with the *reflux ratio* of 3.5, and the *reflux* is a *saturated liquid*

A fractional recovery of 99.4% of *n*-butane is desired in the distillate, and the required fractional recovery of *n*-pentane in the bottom is 99.7%

If the *optimal* feed stage is used, estimate the *distillate* and *bottom compositions* and *flow rates*

Flow chart:



(from "Separation Process Engineering" by Wankat, 2007)

Of these 4 components, the *order* of *volatility* is as follows

$$\text{propane} > n\text{-butane} > n\text{-pentane} > n\text{-hexane}$$

Since the *fractional recovery* of ***n*-butane** (in the *distillate*) is **specified**, ***n*-butane** is the ***key components***

Also, the *fractional recovery* of ***n*-pentane** (in the *bottom*) is **specified**, ***n*-pentane** is another ***key component***

Of these 2 key components (*i.e.* n-butane and n-pentane), ***n*-butane** is the **most volatile** species, while ***n*-pentane** is the **least volatile** one

Thus,

- ***n*-butane** is the *light key* component (**LK**)
- ***n*-pentane** is the *heavy key* component (**HK**)

Hence, **propane** and ***n*-hexane** are the **non-keys (NKs)**

As *propane* is *lighter* (*i.e. more volatile*) than the **LK** (*i.e.* *n*-butane), it is the **LNK**

On the other hand, *n*-hexane is *less volatile* (*i.e. heavier*) than the **HK** (*i.e.* *n*-pentane), it is the **HNK**

Thus, we can **assume** (or **make the first guess**) that

- there is **NO propane** (the **LNK**) in the **bottom**; *i.e.*

$$Bx_{\mathrm{C_3,\ bot}} = 0 \tag{5.17}$$

  or **all** of **propane** ($\mathrm{C_3}$) **appears only** in the **distillate**; *i.e.*

$$Dx_{\mathrm{C_3,\ dist}} = Fz_{\mathrm{C_3}} \tag{5.18}$$

- there is **NO *n*-hexane** (the **HNK**) in the **distillate**; *i.e.*

$$Dx_{\mathrm{C_6,\ dist}} = 0 \tag{5.19}$$

or **all *n*-hexane** (C_6) **comes out only** in the bottom; *i.e.*

$$Bx_{\mathrm{C_6,\ bot}} = Fz_{\mathrm{C_6}} \tag{5.20}$$

From the given **information** regarding **fractional recovery** (in the problem statement), we can write the following equations [for *n*-butane (C_4) and *n*-pentane (C_5)]:

$$Dx_{\mathrm{C_{4,\ dist}}} = \left(0.994\right) Fz_{\mathrm{C_4}} \tag{5.21}$$

$$Bx_{\mathrm{C_{4,\ bot}}} = \left(1 - 0.994\right) Fz_{\mathrm{C_4}} \tag{5.22}$$

$$Bx_{\mathrm{C_{5,\ bot}}} = \left(0.997\right) Fz_{\mathrm{C_5}} \tag{5.23}$$

$$Dx_{\mathrm{C_{5,\ dist}}} = \left(1 - 0.997\right) Fz_{\mathrm{C_5}} \tag{5.24}$$

We also have the following 2 equations:

$$\sum \left(Dx_{i,\ \text{dist}} \right) = D \tag{5.25}$$

$$\sum \left(Bx_{i,\ \text{bot}} \right) = B \tag{5.26}$$

Let's start the calculations with the **distillate**

From Eq. 5.18,

$$Dx_{\text{C}_3,\ \text{dist}} = Fz_{\text{C}_3} = \left(2{,}000\right)\left(0.056\right) = 112$$

and Eq. 5.19,

$$Dx_{\text{C}_6,\ \text{dist}} = 0$$

From Eq. 5.21,

$$\begin{aligned} Dx_{\text{C}_{4,\ \text{dist}}} &= \left(0.994\right) Fz_{\text{C}_4} \\ &= \left(0.994\right)\left(2{,}000\right)\left(0.321\right) \end{aligned}$$

$$Dx_{\text{C}_{4,\ \text{dist}}} = 638.5$$

From Eq. 5.24,

$$\begin{aligned} Dx_{\mathrm{C}_{5,\ \mathrm{dist}}} &= \left(1-0.997\right) Fz_{\mathrm{C}_5} \\ &= \left(1-0.997\right)\left(2,000\right)\left(0.482\right) \end{aligned}$$

$$Dx_{\mathrm{C}_{5,\ \mathrm{dist}}} = 2.89$$

Hence, from Eq. 5.25,

$$\sum\left(Dx_{i,\ \mathrm{dist}}\right) = D = Dx_{\mathrm{C}_{3,\ \mathrm{dist}}} + Dx_{\mathrm{C}_{4,\ \mathrm{dist}}} + Dx_{\mathrm{C}_{5,\ \mathrm{dist}}} + Dx_{\mathrm{C}_{6,\ \mathrm{dist}}}$$

$$\sum\left(Dx_{i,\ \mathrm{dist}}\right) = \boldsymbol{D} = 112 + 638.5 + 2.89 + 0 = \mathbf{753.4}$$

Doing the same for the **bottom**, using Eqs. 5.17 (for propane), 5.20 (for *n*-hexane), 5.22 (for *n*-butane), and 5.23 (for *n*-pentane), yields

- $Bx_{\mathrm{C}_3,\ \mathrm{bot}} = 0$
- $Bx_{\mathrm{C}_6,\ \mathrm{bot}} = Fz_{\mathrm{C}_6} = \left(2,000\right)\left(0.141\right) = 282$

  (note that $z_{\mathrm{C}_6} = 1 - 0.056 - 0.321 - 0.482$ $= 0.141$)

- $Bx_{\mathrm{C_{4,\ bot}}} = \left(1 - 0.994\right) Fz_{\mathrm{C_4}}$
  $= \left(1 - 0.994\right)\left(2,000\right)\left(0.321\right) = 3.85$
- $Bx_{\mathrm{C_{5,\ bot}}} = \left(0.997\right) Fz_{\mathrm{C_5}}$
  $= \left(0.997\right)\left(2,000\right)\left(0.482\right) = 961.1$

Eventually, from Eq. 5.26,

$$\sum\left(Bx_{i,\ \mathrm{bot}}\right) = Bx_{\mathrm{C_{3,\ bot}}} + Bx_{\mathrm{C_{4,\ bot}}} + Bx_{\mathrm{C_{5,\ bot}}} + Bx_{\mathrm{C_{6,\ bot}}}$$

$$\sum\left(Bx_{i,\ \mathrm{bot}}\right) = \boldsymbol{B} = 0 + 3.85 + 961.1 + 282 = \mathbf{1,247.0}$$

Check if $F = D + B$?

$$2,000 = 753.4 + 1,247.0 = 2,000.4\text{: } \textbf{OK!}$$

This means that our **first guess**, with the *assumptions* that

- all **LNK** (*i.e.* **propane** in this Example) goes out only in the *distillate*

- all **HNK** (*i.e.* ***n*-hexane** in this Example) appears only in the *bottom*

seems to **yield** the ***satisfactory*** **answers**

The *compositions* of *each species* in the *distillate* and the *bottom* can be computed as follows

Distillate:

- C_3: $x_{C_3,\text{ dist}} = \dfrac{Dx_{C_3,\text{ dist}}}{D} = \dfrac{112}{753.4} = 0.149$
- C_4: $x_{C_4,\text{ dist}} = \dfrac{Dx_{C_4,\text{ dist}}}{D} = \dfrac{638.5}{753.4} = 0.847$
- C_5: $x_{C_5,\text{ dist}} = \dfrac{Dx_{C_5,\text{ dist}}}{D} = \dfrac{2.89}{753.4} = 0.0038$
- C_6: $x_{C_6,\text{ dist}} = \dfrac{Dx_{C_6,\text{ dist}}}{D} = \dfrac{0}{753.4} = 0$

and

$$\sum x_{i,\text{ dist}} = 0.149 + 0.847 + 0.0038 + 0 = 0.9998$$

Bottom:

- C_3: $x_{C_3,\text{ bot}} = \dfrac{Bx_{C_3,\text{ bot}}}{B} = \dfrac{0}{1,247.0} = 0$
- C_4: $x_{C_4,\text{ bot}} = \dfrac{Bx_{C_4,\text{ bot}}}{B} = \dfrac{3.85}{1,247.0} = 0.0031$
- C_5: $x_{C_5,\text{ bot}} = \dfrac{Bx_{C_5,\text{ bot}}}{B} = \dfrac{961.1}{1,247.0} = 0.771$
- C_6: $x_{C_6,\text{ bot}} = \dfrac{Bx_{C_6,\text{ bot}}}{B} = \dfrac{282}{1,247.0} = 0.226$

and

$$\sum x_{i,\text{ bot}} = 0 + 0.0031 + 0.771 + 0.226 = 1.0001$$

In-class Exercise

Determine the ***non-key*** components, and also indicate that they are *light* or *heavy* **non-keys**

Information: The ***relative volatilities***, with respect to toluene, of the following substances are as follows:

- Benzene = 2.25
- Toluene = 1.00
- Xylene = 0.33
- Cumene = 0.21

System 1: A ternary mixture, where benzene = LK and toluene = HK. ***What is cumene?***

System 2: A ternary mixture, where toluene = LK and xylene = HK. **What is benzene?**

System 3: A four-component system, where toluene = LK and xylene = HK. ***What are benzene and cumene?***

System 4: A four-component system, where benzene = LK and toluene = HK. ***What are xylene and cumene?***

System 5: A 4-component system, where toluene = LK and cumene = HK. ***What are benzene and xylene?***