Single Equilibrium Stages and Flash Calculations
• Single equilibrium stage will be considered here.

• Calculation will be made by combining material balances with phase-equilibrium.

• When a phase change occurs, or when heat effects are large, an energy balance must be added.

• If mass-transfer rates are too slow, or if the time to achieve equilibrium is longer than the contact time, the degree of separation will be less than calculated by the methods used in this part. In that case, stage efficiencies must be introduced into the equations or calculations must be based on mass-transfer rates rather than phase equilibrium.
GIBBS PHASE RULE (phases, components, DOFs)

At physical equilibrium and when only intensive variables are considered, the Gibbs phase rule determines degrees of freedom $\mathcal{F}$

$$\mathcal{F} = C - P + 2$$

$C$ is the number of components, $P$ is the number of phases.

The number of intensive variables is

$$\mathcal{V} = C \cdot P + 2$$

where the 2 refers to temperature and pressure, and $C \cdot P$ is the total number of composition variables (e.g., mole fractions) for components distributed among $P$ phases.

The number of independent equations relating the intensive variables is

$$\mathcal{E} = P + C \cdot (P - 1)$$

where the first term, $P$, refers to the requirement that mole fractions sum to one in each phase, and the second term, $C \cdot (P - 1)$, refers to the number of independent phase-equilibrium equations of the form

$$K_i = \frac{\text{mole fraction of } i \text{ in phase (1)}}{\text{mole fraction of } i \text{ in phase (2)}}$$

where (1) and (2) refer to equilibrium phases.
Independent equations:
\[ C \sum_{i=1}^{C} y_i = 1 \]
\[ C \sum_{i=1}^{C} x_i = 1 \]
\[ K_i = \frac{y_i}{x_i}, \ i = 1 \text{ to } C \]

Independent equations:
Same as for (a) plus
\[ Fz_i = Vy_i + Lx_i \quad i = 1 \text{ to } C \]
\[ Fh_F + Q = Vh_V + Lh_L \]

Figure 4.1 Treatments of degrees of freedom for vapor-liquid phase equilibria: (a) Gibbs phase rule (considers intensive variables only); (b) general analysis (considers both intensive and extensive variables).
FLASH VAPORIZATION AND PARTIAL CONDENSATION

(a) Liquid feed $F, z_i, h_F, T_F, P_F$ and $Q$ through the Heater. $V, y_i, h_V$ and $P_V, T_V$. $P_L, T_L$, $L, x_i, h_L$.

(b) Vapor feed $F, z_i, h_F, T_F, P_F$ through the Partial condenser. $V, y_i, h_V$ and $P_V, T_V$. $P_L, T_L$, $L, x_i, h_L$. 

Diagram shows a flowchart with various components and labels indicating the process parameters.
Table 4.3  Equations for Single-Stage Flash Vaporization and Partial Condensation Operations. Feed mole fractions must sum to one.

<table>
<thead>
<tr>
<th>Equation</th>
<th>Number of Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $P_V = P_L$</td>
<td>1</td>
</tr>
<tr>
<td>(2) $T_V = T_L$</td>
<td>1</td>
</tr>
<tr>
<td>(3) $y_i = K_i x_i$</td>
<td>C</td>
</tr>
<tr>
<td>(4) $F z_i = V y_i + L x_i$</td>
<td>C</td>
</tr>
<tr>
<td>(5) $F = V + L$</td>
<td>1</td>
</tr>
<tr>
<td>(6) $h_F F + Q = h_V V + h_L L$</td>
<td>1</td>
</tr>
<tr>
<td>(7) $\sum_i y_i - \sum_i x_i = 0$</td>
<td>1</td>
</tr>
</tbody>
</table>

$\varepsilon = 2C + 5$

$K_i = K_i \{T_V, P_V, y, x\}$

$h_F = h_F \{T_F, P_F, z\}$

$h_V = h_V \{T_V, P_V, y\}$

$h_L = h_L \{T_L, P_L, x\}$
For the single-stage operation \(2C + 5\) equations listed in Table 4.3 apply. The equations relate the \(3C + 10\) variables \((F, V, L, z_i, y_i, x_i, T_F, T_V, T_L, P_F, P_V, P_L, Q)\) and leave \(C + 5\) degrees of freedom.

Assuming that \(C + 3\) feed variables \(F, T_F, P_F\) and \(C\) values of \(z_i\) are known, two additional variables can be specified for a flash calculation.

The most common sets of specifications are:

| \(T_V, P_V\) | Isothermal flash |
| \(V/F = 0, P_L\) | Bubble-point temperature |
| \(V/F = 1, P_V\) | Dew-point temperature |
| \(T_L, V/F = 0\) | Bubble-point pressure |
| \(T_V, V/F = 1\) | Dew-point pressure |
| \(Q = 0, P_V\) | Adiabatic flash |
| \(Q, P_V\) | Nonadiabatic flash |
| \(V/F, P_V\) | Percent vaporization flash |
EXAMPLE 4.1  Phase Conditions of a Process Stream.

A 100-kmol/h feed consisting of 10, 20, 30, and 40 mol% of propane (3), n-butane (4), n-pentane (5), and n-hexane (6), respectively, enters a distillation column at 100 psia (689.5 kPa) and 200°F (366.5°K). Assuming equilibrium, what fraction of the feed enters as liquid, and what are the liquid and vapor compositions?

\[ K_3 = 4.2, \quad K_4 = 1.75, \quad K_5 = 0.74, \quad K_6 = 0.34, \text{ independent of compositions} \]

\begin{verbatim}
In[8]:= equils = Table[y[i] == K[i] x[i], {i, 1, nc}]
Out[8]= {y_1 == 420 x_1, y_2 == 1.75 x_2, y_3 == 0.74 x_3, y_4 == 0.34 x_4}

In[9]:= bals = Table[z[i] F == x[i] L + y[i] V, {i, 1, nc}]
Out[9]= {10. == L x_1 + V y_1, 20. == L x_2 + V y_2, 30. == L x_3 + V y_3, 40. == L x_4 + V y_4}

In[10]:= sums = {Sum[x[i], {i, 1, nc}] == 1, Sum[y[i], {i, 1, nc}] == 1}
Out[10]= {x_1 + x_2 + x_3 + x_4 == 1, y_1 + y_2 + y_3 + y_4 == 1}

Number of equations: 10
\end{verbatim}
Number of unknowns: 10 \((V, L, x_i, y_i, i = 1,\ldots,4)\)
In[8]:= \[ SR = \text{Table}[(y_i V) / (x_i L), \{i, 1, nc\}]; \]
\[ SF = \text{Table}[(y_i V) / (z_i F), \{i, 1, nc\}]; \]

\text{separation ratio (factor)}

\text{split fraction}

\begin{tabular}{ccccccc}
  \hline
  i & K_i & z_i & x_i & y_i & SR_i & SF_i \\
  \hline
  1 & 420 & 0.1 & 0.000720947 & 0.302798 & 205.61 & 0.99516 \\
  2 & 1.75 & 0.2 & 0.16045 & 0.280788 & 0.856707 & 0.461412 \\
  3 & 0.74 & 0.3 & 0.32803 & 0.242742 & 0.362265 & 0.265928 \\
  4 & 0.34 & 0.4 & 0.510798 & 0.173671 & 0.166446 & 0.142695 \\
  \hline
\end{tabular}
“Traditional” solution method for isothermal flash:

Table 4.4  Rachford–Rice Procedure for Isothermal-Flash Calculations When K-Values Are Independent of Composition

<table>
<thead>
<tr>
<th>Steps</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $T_L = T_V$</td>
<td></td>
</tr>
<tr>
<td>(2) $P_L = P_V$</td>
<td></td>
</tr>
<tr>
<td>(3) Solve</td>
<td>$f{\Psi} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$</td>
</tr>
<tr>
<td>for $\Psi = V/F$, where $K_i = K_i(T_V, P_V)$.</td>
<td></td>
</tr>
<tr>
<td>(4) $V = F\Psi$</td>
<td></td>
</tr>
<tr>
<td>(5) $x_i = \frac{z_i}{1 + \Psi(K_i-1)}$</td>
<td></td>
</tr>
<tr>
<td>(6) $y_i = \frac{z_iK_i}{1 + \Psi(K_i-1)} = x_iK_i$</td>
<td></td>
</tr>
<tr>
<td>(7) $L = F - V$</td>
<td></td>
</tr>
<tr>
<td>(8) $Q = h_VV + h_LL - h_FF$</td>
<td></td>
</tr>
</tbody>
</table>

- Method is used in process simulators
- General software packages are able to solve the flash problems
At the **bubble point**

\[ \sum_{i=1}^{n_c} p_i = p \rightarrow \sum_{i=1}^{n_c} x_i p_i^0 = p \rightarrow \sum_{i=1}^{n_c} x_i K_i = 1 \equiv f(T) \]

At the **dew point**

\[ \sum_{i=1}^{n_c} x_i = 1 \rightarrow \sum_{i=1}^{n_c} \frac{y_i p_i^0}{p_i} = 1 \rightarrow \sum_{i=1}^{n_c} \frac{y_i}{K_i} = 1 \equiv g(T) \]

\[ K_i = \frac{p_i^0}{p} \quad \ln p_i^0 = A_i - \frac{B_i}{C_i} + T \]

For \( T=\text{const.} \) the above equations allow for (easy?) evaluations of the **bubble point pressure** and the **dew point pressure**
ADIABATIC FLASH

• When the pressure of a liquid stream is reduced adiabatically across a valve, an adiabatic flash \((Q = 0)\) calculation is made to determine the resulting phases, temperature, compositions, and flow rates for a specified downstream pressure.

• The calculation can be made by applying the isothermal-flash calculation procedure in an iterative manner.

• First a guess is made of the flash temperature, \(T_V\). Then \(V/F, V, x, y,\) and \(L\) are determined, as for an isothermal flash. The guessed value of \(T_V\) (equal to \(T_L\)) is next checked by an energy balance with \(Q=0\).

• Enthalpies are computed at \(T_V=T_L\). The procedure is tedious because it involves inner-loop iteration on \(V/F\) and outer-loop iteration on \(T_V\).