Batch Distillation

SHR Chapter 13
Simple Binary Batch Distillation Analysis

Light key mole balance:
\[ \frac{d(Wx)}{dt} = -Dy \]
\[ W \frac{dx}{dt} + x \frac{dW}{dt} = -Dy \]

Overall mole balance:
\[ \frac{dW}{dt} = -D \]

- \( D \) Distillate molar flow rate
- \( W \) Moles of “residue” in the still
- \( x \) Mole fraction of light key in the still (assumed spatially homogeneous)
- \( y \) Mole fraction of light key in the distillate (assumed spatially homogeneous)

To integrate the LHS term, we need to know \( y(x) \).
Consider a single-stage with no reflux.

Option 1: assume that $K = \frac{y}{x}$ is constant.

\[
\int_{x_0}^{x} \frac{dx}{y - x} = \int_{W_0}^{W} \frac{dW}{W} = \ln \frac{W}{W_0}
\]

\[
\frac{1}{K - 1} \ln \left( \frac{x}{x_0} \right) = \ln \left( \frac{W}{W_0} \right) \quad \text{(constant } K) \]

Option 2: assume that $\alpha$ is constant.

\[
\alpha \equiv \frac{K_A}{K_B} = \frac{y_A/x_A}{y_B/x_B} = \frac{y/x}{(1-y)/(1-x)} \quad \Rightarrow \quad y = \frac{\alpha x}{1 + x (\alpha - 1)}
\]

\[
\int_{x_0}^{x} \left( \frac{1 + x (\alpha - 1)}{\alpha x} - x \right)^{-1} dx = \ln \left( \frac{W}{W_0} \right) \quad \Rightarrow \quad \ln \left( \frac{W_0}{W} \right) = \frac{1}{\alpha - 1} \left[ \ln \left( \frac{x_0}{x} \right) + \alpha \ln \left( \frac{1 - x}{1 - x_0} \right) \right] \quad \text{(constant } \alpha) \]

Option 3: if $T$-$x$-$y$ data are available, integrate numerically using the trapezoid rule.
Example: Constant Boilup

A batch still is loaded with 100 kmol of a binary mixture of 50 mol% benzene in toluene. As a function of time, make plots of:
(a) still temperature,
(b) instantaneous vapor composition,
(c) still-pot composition, and
(d) average total-distillate composition.

Assume a constant boilup rate, 10 kmol/h of product, and a constant α of 2.41 at a pressure of 101.3 kPa (1 atm).

Total amount distilled: \( W_0 - W \)
Amount of light key distilled: \( x_0 W_0 - x W \)

\[ y_{\text{avg}} = \frac{x_0 W_0 - x W}{W_0 - W} \]

average distillate composition (see SHR eq. (13-6))

From the \( T-x-y \) data in SHR Table 13.1, we get \( T \) from \( x \).

\[ \ln \left( \frac{W_0}{W} \right) = \frac{1}{\alpha - 1} \left[ \ln \left( \frac{x_0}{x} \right) + \alpha \ln \left( \frac{1 - x}{1 - x_0} \right) \right] \]

It is easier to solve for \( W(x) \) than \( x(W) \).

How do we connect \( W \) and \( x \) to \( t \)?

\[ \frac{dW}{dt} = -D \quad \text{constant boilup...} \]

\[ W = W_0 - Dt \Rightarrow t = \frac{W_0 - W}{D} \]

From the \( T-x-y \) data in SHR Table 13.1, we get \( T \) from \( x \).
Example: Using Tabular Data

A batch still is loaded with 100 kmol of a binary mixture of 50 mol% benzene in toluene. As a function of time, make plots of:

(a) still temperature,
(b) instantaneous vapor composition,
(c) still-pot composition, and
(d) average total-distillate composition.

Assume a constant boilup rate, 10 kmol/h of product, and use the $T$-$x$-$y$ data in SHR Table 13.1.

\[
\int_{x_0}^{x} \frac{dx}{y - x} = \ln \frac{W}{W_0}
\]

Different approach to get this term. Otherwise it is the same as the last example.

\[
\int_{a}^{b} f(x) \, dx \approx \frac{b-a}{2} [f(a) + f(b)]
\]

trapz in matlab...

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<th>$y$</th>
<th>$T$</th>
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<tr>
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</table>

$x$ decreases in time from 0.5.
Batch Distillation with Constant Reflux Ratio

Assumptions:
• McCabe-Thiele analysis (see notes on binary distillation)
• Total condenser
• Constant molar overflow
• Only heat transfer is in condenser and reboiler (not in the rectifying section)
• Constant $V$ and $R$ (implies constant $L$ and $D$)

\[
\int_{x_{W_0}}^{x_W} \frac{dx_W}{x_D - x_W} = \ln \frac{W}{W_0}
\]

came from the mole balance (see slide 2)

$x_D$ is a nontrivial function of $x_W$, depending on 
# stages, reflux ratio, equilibrium, etc.
That means that this integral is not easy to get!

\[
\frac{dW}{dt} = L - V = -D
\]

\[
\int_{W_0}^{W} dW = (L - V) t
\]

\[
W = W_0 + (L - V) t
\]

\[
= W_0 + V \left( \frac{L}{V} - 1 \right) t
\]

\[
= W_0 - \frac{V}{R + 1} t
\]

Time to reach amount $W$ in still.

Concept:
• Use McCabe-Thiele to get the relationship between $x_D$ and $x_W$.
• Given the graphically-obtained integrand, carry out the integration to find $W(x_W)$.
• Choose $x_W$ - find $W$ - find $t$. 
McCabe-Thiele to get \((x_D - x_W)\)

Assume that the number of theoretical stages \((N_t)\) and the reflux ratio \((R)\) are known.

1. Choose \(x_W\).
2. Construct an operating line with the prescribed \(R\) such that in \(N_t\) stages, we hit the intersection of the operating line and the 45° line. This defines \(x_D\) for the \(x_W\) chosen in step 1.
3. Repeat steps 1-2 for the desired range of \(x_W\), choosing “enough” points to do step 4.
4. Numerically integrate (trapezoid rule) to find \(\ln(W/W_0)\).
5. From \(W\), find \(t\).

\[
\frac{L}{V} = \frac{R}{R+1} \quad \int_{x_{W_0}}^{x_W} \frac{dx_W}{x_D - x_W} = \ln \frac{W}{W_0}
\]

Calculate average distillate composition over time \(t\) as before:

\[
x_D^{avg} = \frac{x_{W_0} W_0 - x_W W}{W_0 - W}
\]
Batch Distillation with Constant $x_D$

**Idea:** constant $V$ and vary $R$ in time to obtain a desired $x_D$.

- More difficult than constant $R$, but typically more desirable.
- Implies that $D$ is changing in time.

\[
x_{D}^{\text{avg}} = \frac{x_W W_0 - x_W W}{W_0 - W} \Rightarrow W = W_0 \left[ \frac{x_D - x_W}{x_D - x_W} \right]
\]

\[
dW/dt, \text{ assume constant } x_D \text{ and rearrange...}
\]

\[
\frac{dW}{dt} = W_0 \frac{x_D - x_W}{(x_D - x_W)^2} \frac{dx_W}{dt}
\]

\[
(V - L) = W_0 \frac{x_D - x_W}{(x_D - x_W)^2} \frac{dx_W}{dt}
\]

\[
dt = VW_0 (x_D - x_W_0) \frac{dx_W}{(1 - \frac{L}{V}) (x_D - x_W)^2}
\]

Recall that $x_D$ is known (constant) and $V$ is constant, but $L/V$ is changing depending on $x_W$.

\[
t = VW_0 (x_D - x_W_0) \int_{x_W_0}^{x_W} \frac{dx_W}{(1 - \frac{L}{V}) (x_D - x_W)^2}
\]

Use McCabe-Thiele to get values of the integrand graphically.
1. Choose $x_W$.  
2. Construct an operating line with $R$ such that in $N_t$ stages, we hit the intersection of the operating line and the 45º line. This defines $R$ for the $x_W$ chosen in step 1.  
3. Repeat steps 1-2 for the desired range of $x_W$, choosing “enough” points to do step 4.  
4. Numerically integrate (trapezoid rule) to find $t$ for a given $x_W$.  

$$t = V W_0 (x_D - x_{W_0}) \int_{x_{W_0}}^{x_W} \frac{dx_W}{(1 - \frac{L}{V}) (x_D - x_W)^2}$$  

$$W = W_0 \left[ \frac{x_D - x_{W_0}}{x_D - x_W} \right]$$