**Reaction with phase change, conducted in a PFR**

e.g. 3.10 (slightly modified)

Consider a gas phase reaction, where one of the products can also condense at the operating conditions. This is done in a PFR, with negligible pressure drop and at isothermal conditions.

\[ A_{(g)} + 2B_{(g)} \rightarrow C_{(g)} + D_{(s,l)} \]

The vapor pressure of D is given by \( P_V = 16 \text{ kPa} \). The operating pressure is 101.3 kPa.

Let us say the reaction is a first order reaction with \( k = 0.1 \text{ s}^{-1} \). The inlet conditions are \( F_{A0} = 10 \text{ mol/s}, F_{B0} = 20 \text{ mol/s}, Q = 1 \text{ m}^3/\text{s} \).

(i) Find the conversion \( x \) when condensation begins

(ii) Write \( C_A, C_B \), etc in terms of conversion.

(iii) What is the volume of reactor needed to get 80% conversion?

**Ans:**

Let us first write the stoichiometric table. Here \( X_c \) denotes the conversion at the point of condensation.

<table>
<thead>
<tr>
<th>Species</th>
<th>Initial</th>
<th>At any ( x \leq X_c )</th>
<th>At any ( x \geq X_c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>( F_{A0} )</td>
<td>( F_{A0} (1-x) )</td>
<td>( F_{A0} (1-x) )</td>
</tr>
<tr>
<td>B</td>
<td>( 2 F_{A0} )</td>
<td>( 2 F_{A0} (1-x) )</td>
<td>( 2 F_{A0} (1-x) )</td>
</tr>
<tr>
<td>C</td>
<td>0</td>
<td>( F_{A0} x )</td>
<td>( F_{A0} x )</td>
</tr>
<tr>
<td>D (gas)</td>
<td>0</td>
<td>( F_{A0} x )</td>
<td>( Y_D F_{T,g} )</td>
</tr>
<tr>
<td>D (liquid)</td>
<td>0</td>
<td>0</td>
<td>( F_{A0} x - Y_D F_{T,g} )</td>
</tr>
<tr>
<td>D (Total)</td>
<td>0</td>
<td>( F_{A0} x )</td>
<td>( F_{A0} x )</td>
</tr>
<tr>
<td>Total (gas)</td>
<td>3 ( F_{A0} )</td>
<td>( F_{A0} (3-x) )</td>
<td>( Y_D F_{T,g} + 3 F_{A0} - 2 F_{A0} x )</td>
</tr>
<tr>
<td>Total (liquid)</td>
<td>0</td>
<td>0</td>
<td>( F_T - F_{T,g} )</td>
</tr>
<tr>
<td>Total</td>
<td>3 ( F_{A0} )</td>
<td>( F_{A0} (3-x) )</td>
<td>( F_{A0} (3-x) )</td>
</tr>
</tbody>
</table>

Note that the mole fraction of D in the gas phase is given by

\[ y_D = \frac{F_{D,g}}{F_{T,g}} \]

Before condensation, all the species are in the gas phase. After condensation, part of D is in the liquid phase.

At condensation, the partial pressure of D \( P_D = P_V = 16 \text{ kPa} \)

\[ y_D = \frac{16}{101.3} = \frac{F_{A0} x}{F_{A0} (3-x)} = \frac{F_{A0} x - y_D F_{T,g}}{y_D F_{T,g} + 3 F_{A0} - 2 F_{A0} x} \]

Implying \( X_c = 0.41 \)
At that point, $F_{D,1} = F_{T,1} = 0$. After that, it will increase. 

i.e. At the point of condensation $F_{A_0}(3-x_c) - \frac{F_{A_0}(3-2x_c)}{1-y_D} = 0$. We can re-arrange this also and get $X_c$.

**Before condensation**

$$C_A = \frac{F_A}{Q} = \frac{F_{A_0}(1-x)}{Q_0(1+\varepsilon x)} = \frac{C_{A_0}(1-x)}{(1-0.33x)}$$

Here, $Q = \frac{F_{T_0}RT}{P} = \frac{F_TQ_0}{F_{T_0}} = Q_0(1+\varepsilon x)$ Please note that this is before condensation.

Here $\varepsilon = \frac{2-3}{3} = -0.33$

**After condensation:**

$Q = \frac{F_{T,s}RT}{P}$. Note that the liquid phase flow rate will be negligible because the liquid density is typically much more than the gas density.

We have to calculate the total molar flow rate in gas phase. This is obtained by rearranging the equation

$F_{T,s} = y_D F_{T,s} + 3F_{A_0} - 2F_{A_0}x$

$F_{T,s} = \frac{F_{A_0}(3-2x)}{1-y_D}$

Therefore,

$$Q = \frac{F_{T,s}RT}{P} = \frac{F_{A_0}(3-2x)RT}{1-y_D}$$

We can use the initial conditions to get $\frac{Q_0}{F_{T_0}} = \frac{RT}{P}$

Therefore,

$$Q = \frac{F_{A_0}(3-2x)Q_0}{1-y_D} F_{T_0} = \frac{F_{A_0}(3-2x)}{1-y_D} \frac{Q_0}{3F_{A_0}} = \frac{Q_0(3-2x)}{3(1-y_D)}$$

The concentration can be written as

$$C_A = \frac{F_A}{Q} = \frac{F_{A_0}(1-x)}{Q_0(3-2x)} = \frac{3C_{A_0}(1-x)(1-y_D)}{(3-2x)}$$
To find the PFR volume, we need to use the design equation \( \frac{dF_A}{dV} = r_A \). Since the expression for \( C_A \) and hence \( r_A \) change during condensation, we need to write this in two parts.

\[
\frac{dF_A}{dV} = r_A \text{ becomes } \frac{F_{A0}dx_A}{dV} = kC_A
\]

Re-arranging

\[
\frac{F_{A0}dx_A}{kC_A} = dV
\]

\[
\int_0^{0.8} \frac{F_{A0}dx_A}{kC_A} = \int_0^V dV = V = \int_0^{0.41} \frac{F_{A0}dx_A}{kC_A} + \int_{0.41}^{0.8} \frac{F_{A0}dx_A}{kC_A}
\]

First part:

\[
10 \int_0^{0.41} \frac{(0.67)dx_A}{(1-x)} + 3.3 \int_0^{0.41} dx_A = -6.7 \ln(1-x)|_{0.41}^{0.41} + 3.3 \times 0.41 = 4.88 \text{ m}^3
\]

Second part

\[
10 \int_{0.41}^{0.8} \frac{(3-2x)dx}{kC_A (1-x)} = \frac{10}{3 \times 0.1 \times 10 \times (1-0.16)} \int_{0.41}^{0.8} (3-2x)dx
\]

\[
= 3.97 \times \left( \frac{1}{1-x} + 2 \right) dx = 3.97 \times \left( -\ln(1-x) + 2x \right)_{0.41}^{0.8} = 3.97 \times [3.21 - 1.35] = 7.4 \text{ m}^3
\]

Total volume needed is roughly 12.28 m\(^3\).