Introduction to Reactor Design, 3K4

Multiple reactions in a PFR: *the algorithm to set up the equations*

Example

Formaldehyde, HCHO, decomposes to formic acid, HCOOH, on a catalyst.

1	$\text{HCHO} + \frac{1}{2}\text{O}_2 \xrightarrow{k_1} \text{HCOOH}$
2	$2\text{HCHO} \xrightarrow{k_2} \text{HCOOCH}_3$
3	$\text{HCOOH} \xrightarrow{k_3} \text{CO} + \text{H}_2\text{O}$
4	$\text{HCOOCH}_3 + \text{H}_2\text{O} \xrightarrow{k_4} \text{CH}_3\text{OH} + \text{HCOOH}$
1	$\text{A} + \frac{1}{2}\text{B} \xrightarrow{k_1} \text{C}$
2	$2\text{A} \xrightarrow{k_2} \text{D}$
3	$\text{C} \xrightarrow{k_3} \text{E} + \text{W}$
4	$\text{D} + \text{W} \xrightarrow{k_4} \text{G} + \text{C}$

$F_{A0} = 10\,\text{mol.s}^{-1}$, $F_{B0} = 5\,\text{mol.s}^{-1}$, $q_0 = 100\,\text{L.s}^{-1}$, $W = 1000\,\text{kg}$ and $C_{T0} = 1.0\,\text{mol.L}^{-1}$

At 300K, we are given $k_1 = 0.014\,\dfrac{\text{L}^{0.5}}{\text{mol}^{0.5}\text{s}}$; $k_2 = 0.007\,\text{L.mol}^{-1}\text{.s}^{-1}$; $k_3 = 0.014\text{s}^{-1}$; and that $k_4 = 0.45\,\text{L.mol}^{-1}\text{.s}^{-1}$. Initially consider no effects due to pressure drop.

AIM:

1. Plot the profiles along the reactor of the gas concentrations.
2. Plot the profiles along the reactor of yield of HCOOH and selectivity of HCOOH with respect to CO and methyl formate, HCOOCH_3.
3. What will happen to yield and selectivity if we increase the oxygen to formaldehyde feed ratio?
4. Take pressure drop effects into account, using $\alpha = 0.002\,\text{L}^{-1}$. How do these profiles change now?