Midterm 1 Solutions

Problem 1

In order to solve for $C_{A,2}$, $C_{B,2}$, and $C_{P,2}$, in the outlet stream of tank 2, the concentrations of *A* and *B* entering tank 2, $C_{A,1}$ and $C_{B,1}$ respectively, must be found.

First, do a mass balance on species A in tank 1:

$$\frac{dn_A}{dt} = \dot{n}_{A,\text{in}} - \dot{n}_{A,1} + \int_{CV} r_{A,1}(\underline{x}, t)dV \quad (1)$$

Process is at steady state. The tank is well-mixed such that reaction rate does not depend on position and $C_{A,1} = C_A$ in the tank.

$$0 = C_{A,\text{in}}Q - C_{A,1}Q - k_1 C_{A,1} V \quad (2)$$

Write in terms of tau:

$$0 = C_{A,\text{in}} - C_{A,1} - k_1 C_{A,1} \tau \quad (3)$$

$$0 = C_{A,\text{in}} - C_{A,1}(1 + k_1)\tau \quad (4)$$

$$C_{A,1} = \frac{C_{A,\text{in}}}{(1 + k_1)\tau} = \mathbf{1}\frac{\boldsymbol{mol}}{\boldsymbol{L}} \quad (5)$$

Then, a mass balance on species B in tank 1 using the same assumptions listed above:

$$\frac{dn_B}{dt} = \dot{n}_{B,\text{in}} - \dot{n}_{B,1} + \int_{CV} r_{B,1}(\underline{x}, t)dV \quad (6)$$

$$0 = -C_{B,1}Q + k_1 C_{A,1} V \quad (7)$$

$$0 = -C_{B,1} + k_1 C_{A,1} \tau \quad (8)$$

$$C_{B,1} = k_1 C_{A,1} \tau = \mathbf{1}\frac{\boldsymbol{mol}}{\boldsymbol{L}} \quad (9)$$

Now, the second tank is the control volume and mass balances on species A, B, and P are used.

Species mass balance on species A in tank 2:

$$\frac{dn_A}{dt} = \dot{n}_{A,1} - \dot{n}_{A,2} + \int_{CV} r_{A,2}(\underline{x}, t)dV \quad (10)$$

$$0 = C_{A,1}Q - C_{A,2}Q - k_2 C_{A,2} V \quad (11)$$

$$0 = C_{A,1} - C_{A,2} - k_2 C_{A,2} \tau \quad (12)$$

$$0 = C_{A,1} - C_{A,2}(1 + k_2)\tau \quad (13)$$

$$C_{A,2} = \frac{C_{A,1}}{(1 + k_2)\tau} = \frac{\mathbf{1}}{\mathbf{3}}\frac{\boldsymbol{mol}}{\boldsymbol{L}} \quad (14)$$

Species mass balance on species B in tank 2:

$$\frac{dn_B}{dt} = \dot{n}_{B,1} - \dot{n}_{B,2} + \int_{CV} r_{B,2}(\underline{x}, t)dV \quad (10)$$

$$0 = C_{B,1}Q - C_{B,2}Q - k_3 C_{B,2} V \quad (11)$$

$$0 = C_{B,1} - C_{B,2}(1 + k_3\tau) \tag{12}$$

$$C_{B,2} = \frac{C_{B,1}}{(1 + k_3)\tau} = \frac{\mathbf{1}}{\mathbf{4}}\frac{\boldsymbol{mol}}{\boldsymbol{L}} \tag{13}$$

Species mass balance on species P in tank 2:

$$\frac{dn_P}{dt} = \dot{n}_{P,1} - \dot{n}_{P,2} + \int_{CV} r_{P,2}(\underline{x}, t)dV + \int_{CV} r_{P,3}(\underline{x}, t)dV \tag{14}$$

$$0 = -C_{P,2}Q + k_2C_{A,2}V + k_3C_{B,2}V \tag{15}$$

$$0 = -C_{P,2} + k_2C_{A,2}\tau + k_3C_{B,2}\tau \tag{16}$$

$$C_{P,2} = k_2C_{A,2}\tau + k_3C_{B,2}\tau = \frac{\mathbf{17}}{\mathbf{12}}\frac{\boldsymbol{mol}}{\boldsymbol{L}} \tag{17}$$

Problem 2

a. First, do an overall mass balance on the control volume (the entire tank and MOF bed):

$$\frac{dm}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}} \tag{1}$$

Since no flows enter or exit the system,

$$\frac{dm}{dt} = 0 \tag{2}$$

$$M_w \frac{dn}{dt} = 0 \tag{3}$$

$$\frac{dn}{dt} = 0 \tag{4}$$

$$N_0 = n_{\text{MOF}}(t) + n_{\text{Gas}}(t) \tag{5}$$

Do a mass balance on the gas phase to solve for $n_{\text{Gas}}(t)$:

$$\frac{dn_{\text{Gas}}}{dt} = \dot{n}_{\text{Gas,in}} - \dot{n}_{\text{Gas,out}} + \dot{G}_i \tag{6}$$

The entire tank and MOF bed are the control volume, so there are no flows in or out of the system.

$$\frac{dn_{\text{Gas}}}{dt} = -kbP \tag{7}$$

Use ideal gas law to write pressure in terms of moles:

$$\frac{dn_{\text{Gas}}}{dt} = -\left(\frac{kbRT}{V}\right) n_{\text{Gas}} \tag{8}$$

$$\int_{N_0}^{n_{\text{Gas}}(t)} \frac{dn_{\text{Gas}}}{n_{\text{Gas}}} = \int_0^t -\left(\frac{kbRT}{V}\right) dt \tag{9}$$

$$\ln n_{\text{Gas}}(t) - \ln N_0 = -\left(\frac{kbRT}{V}\right) t \tag{10}$$

$$n_{\text{Gas}}(t) = N_0 e^{-\left(\frac{kbRT}{V}\right)t} \tag{11}$$

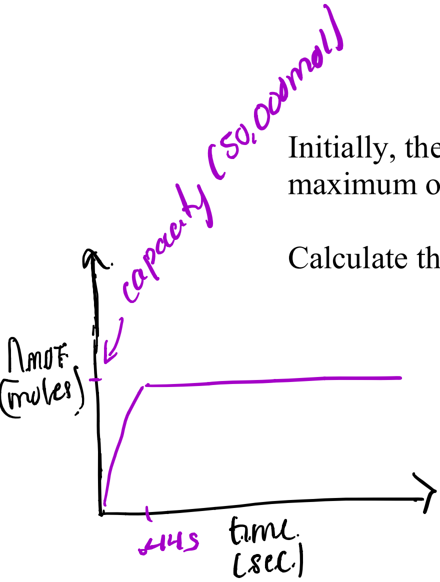
Then, use equation 5 to solve for $n_{\text{MOF}}(t)$:

$$n_{\text{MOF}}(t) = N_0 - N_0 e^{-\left(\frac{kbRT}{V}\right)t} \tag{12}$$

$$\boldsymbol{n_{\text{MOF}}(t) = N_0\left(1 - e^{-\left(\frac{kbRT}{V}\right)t}\right)} \tag{13}$$

b. First calculate the total number of moles that the MOF can adsorb:

$$(10{,}000kg\ MOF)\left(\frac{5mmol\ CH_4}{g\ MOF}\right)\left(\frac{1000g}{kg}\right)\left(\frac{mol}{1000mmol}\right) = 50{,}000\ moles\ CH_4 \tag{14}$$



Initially, there are 75,000 moles of methane in the tank, but the MOF bed can adsorb a maximum of 50,000 moles of methane.

Calculate the time at which maximum capacity is reached using equation 13:

$$n_{\text{MOF}}(t) = 50{,}000 = N_0\left(1 - e^{-\left(\frac{kbRT}{V}\right)t}\right) \quad (15)$$

$$\frac{50{,}000}{75{,}000} = \left(1 - e^{-(2*0.5*8.314*300/1000)t}\right) \quad (16)$$

$$\frac{2}{3} = \left(1 - e^{-2.494t}\right) \quad (17)$$

$$\ln\left(\frac{1}{3}\right) = -2.494t \quad (18)$$

$$\boldsymbol{t = 0.44s} \quad (\mathbf{19})$$

c. Calculate the pressure of methane left in the tank. From part b, we know 25,000 moles are left in the tank.

$$PV = n_{gas}RT \quad (20)$$

$$P = \frac{n_{gas}RT}{V} \quad (21)$$

$$P = \frac{(25{,}000mol)(8.314\frac{m^3 \cdot Pa}{mol \cdot K})(300K)}{1000\ m^3} \quad (22)$$

$$\boldsymbol{P = 62{,}360\ Pa} \quad (\mathbf{23})$$