Question 1 (30 points)

(a) 9 points [each mass balance – 4.5]

The mass balances for A and B are (with $K_f = k_1, K_b = k_2$):

$$V \cdot \frac{dC_A}{dt} = C_{Ai}q - C_A q - 2\left[C_A^2 K_f V - K_b C_B C_C V\right] \quad (1)$$
$$V \cdot \frac{dC_B}{dt} = -C_B q + C_A^2 K_f V - K_b C_B C_C V - K_m A_m C_B \quad (2)$$

Note that we have a factor of 2 for the mass balance for A since we need to multiply the net flux $[v_f - v_b]$ by the stoichiometric coefficient.

(b) 9 points [approach – 7.5 , each st. st. concentration – 0.5]

At a steady state, the rates of change of the concentrations are 0. The mass balance for A becomes

$$0 = -\frac{q}{V}C_A + \frac{q}{V}C_{Ai} - 2\left[C_A^2 K_f - K_b C_B C_C\right]$$
$$\Rightarrow K_f C_A^2 - K_b C_B C_C = \frac{q}{2V}(C_{Ai} - C_A) \quad (3)$$

Similarly, the mass balance for B becomes:

$$0 = -\frac{q}{V}C_B + C_A^2 K_f - K_b C_B C_C - \frac{K_m A_m C_B}{V}$$
$$\Rightarrow K_f C_A^2 - K_b C_B C_C = \frac{1}{V}(q C_B + K_m A_m C_B)$$
$$\Rightarrow K_f C_A^2 - K_b C_B C_C = \frac{1}{V}(q + K_m A_m)C_B \quad (4)$$

If we equate the LHS of 3 and 4 and plug in the relationship that $C_A = 5C_B$, we get

$$\frac{1}{V}(q + K_m A_m)C_B = \frac{q}{2V}(C_{Ai} - 5C_B)$$
$$\Rightarrow 2 * (0.25 + 1.5 * 4)C_B = 0.25(10 - 5C_B)$$
$$\Rightarrow 2 * 6.25\, C_B = 2.5 - 1.25 C_B$$
$$\Rightarrow 13.75 C_B = 2.5$$
$$\Rightarrow C_B = \frac{2.5}{13.75}\ ; C_A = \frac{12.5}{13.75}$$

Plugging in these values into 3, we get:

$$0.5 * \frac{12.5}{13.75} * \frac{12.5}{13.75} - 2.5 * \frac{2.5}{13.75} * C_C = \frac{0.25}{2 * 3} * \left(10 - \frac{12.5}{13.75}\right)$$
$$\Rightarrow 12 * \frac{12.5}{13.75} * \frac{12.5}{13.75} - 60 * \frac{2.5}{13.75} * C_C = \left(10 - \frac{12.5}{13.75}\right)$$
$$\Rightarrow 12 * \frac{12.5}{13.75} * \frac{12.5}{13.75} - 60 * \frac{2.5}{13.75} * C_C = \left(\frac{137.5 - 12.5}{13.75}\right)$$
$$\Rightarrow 12 * \frac{12.5 * 12.5}{13.75} - 60 * 2.5 * C_C = 125$$
$$\Rightarrow 136.36 - 150 * C_C = 125$$
$$\Rightarrow C_C = 0.07575$$

(c) 9 points [linearization – 6 , A_m linearization - 3]

The linearized equations are as follows (tilde denotes the deviations). Note that we also have to linearize around the membrane area since it is now a variable. Therefore, we have

$$\frac{d\widetilde{C_A}}{dt} = -\frac{q}{V}\widetilde{C_A} - 4K_f C_A^{ss}\widetilde{C_A} + 2K_b C_C^{SS}\widetilde{C_B} + 2\, K_b C_B^{SS}\widetilde{C_C}$$
$$\frac{d\widetilde{C_B}}{dt} = -\frac{q}{V}\widetilde{C_B} + 2K_f C_A^{ss}\widetilde{C_A} - K_b C_C^{SS}\widetilde{C_B} - K_b C_B^{SS}\widetilde{C_C} - K_m A_m^{ss}\widetilde{C_B} - K_m C_B^{SS}\widetilde{A_m}$$

(d) 3 points

We have a form of the equation $\frac{dx}{dt} = \boldsymbol{Ax}(t) + \boldsymbol{Bu}(t)$

Here $\boldsymbol{A}$ is the nxn and $\boldsymbol{B}$ nxp state space matrices, with $\boldsymbol{x}$ being the nx1 vector of states, and $\boldsymbol{u}$ the input px1 vector. When we apply the Laplace transform to this equation, we get

$$sX(s) - \boldsymbol{x}(0) = \boldsymbol{A}X(s) + \boldsymbol{B}U(s)$$

The transfer functions are always defined for $\boldsymbol{x}(0) = 0$, therefore the transfer function X(s)/U(s) which will give us the dependence of the concentrations on the area of the membrane is derived as follows:

$$sX(s) = \boldsymbol{A}X(s) + \boldsymbol{B}U(s) \rightarrow (sI - \boldsymbol{A})X(s) = \boldsymbol{B}U(s)$$

$$\frac{X(s)}{U(s)} = (sI - \boldsymbol{A})^{-1}\boldsymbol{B}$$