Exercise 1: Answer guide

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1. (a) Extensive variables depend on the size or amount of the system (e.g. mass, volume) while intensive variables do not (temperature, pressure).

   (b) In case 1 the entire tank is lumped together. Thus one will only describe the overall composition, temperature, etc. of the tank, and the liquid and vapour flows out of the tank. In case 2 the phases are considered separately, hence one will have terms for the composition, temperature etc. in the two phases. Case 2 is more detailed than case 1.

   (c) Instead of explicitly modelling the transport between phases we can instead assume that there is phase equilibrium. Assuming phase equilibrium greatly simplifies the model. If the simplified model matches reality "well-enough", e.g. phase equilibrium is established quickly, or if this level of detail is not required, then the assumption is reasonable.

   (d) Yes. This would mean one only the energy and temperature equal throughout the tank, and only an overall energy balance would be used.

   (e) Case 2 would not describe the system as the composition in the stagnant region could be different to that of the bulk fluid, leading to differences in the output liquid concentration.

   (f) There are many possible answers – one example: if the energy balance between the wall and the inside of the tank needs to be taken into account, then one would define the tank wall as another volume.

2. (a)

$$V\frac{dC_A}{dt} = F_{in}(C_{A,in} - C_A) - kC_AV$$

where V was the volume of reactants $[m^3]$, F was the volumetric flowrate $[m^3s^{-1}]$, kC_A was the reaction rate $[mols^{-1}m^3]$, C_A was the feed concentration $[mols^{-1}m^{-3}]$. We can rearrange this equation by dividing through by the volume V, to give:

$$\frac{dC_A}{dt} = \frac{(C_{A,in} - C_A)}{\tau} - kC_A$$

where τ ha the units of $[s]$, being a characteristic time constant for the reactor. We can now apply the following normalizations:

$$\bar{C}_A = \frac{C_A}{C_{A,in}}$$

$$\bar{t} = \frac{t}{\tau}$$

we can now substitute the variables for the variables on the original equation, which on rearranging gives:

$$\frac{d\bar{C}_A}{d\bar{t}} = 1 - \bar{C}_A - k\tau\bar{C}_A$$

(b) $D = k\tau$, This is called the Damköhler number , it controls the dynamics of the reactor.

3. (a) Diagram should indicate sensor and fluid. Ideally also an arrow or other indication of energy transfer between the fluid and sensor.

   (b) The sensor and fluid are control volumes. As there is no mass transfer the only extensive variable of interest is energy.

   (c) Assumptions: Fluid and sensor are homogeneous, the overall heat transfer between bulk fluid and sensor can be described by a $hA(T - T_{fluid})$ with a constant heat transfer coefficient and interfacial area. Proceeding from an energy balance:

$$\begin{aligned}\frac{dU}{dt} &= Q \\ \frac{dMc_PT}{dt} &= Mc_P\frac{dT}{dt} = hA(T - T_{fluid})\end{aligned}$$

   (d)

$$\begin{aligned}\frac{dT}{dt} &= \frac{hA}{Mc_P}(T - T_{fluid}) \\ dT &= T_{fluid}d\theta \\ dt &= \frac{Mc_P}{hA}d\tau \\ \frac{hAT_{fluid}}{Mc_P}\frac{d\theta}{d\tau} &= \frac{hA}{Mc_P}(T_{fluid}\theta - T_{fluid}) \\ \frac{d\theta}{d\tau} &= (\theta - 1)\end{aligned}$$