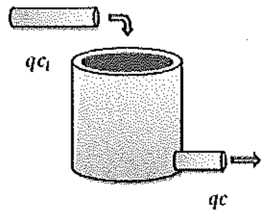
Worksheet #2: Scaling

Consider a chemical reactor tank with flow rate q, volume V, incoming concentration of reactant c_i. We stir the tank so concentration inside $c(t)$ is uniform, so (chemical) mass inside is $Vc(t)$. While inside the tank, the reactant decays at a rate k. In other words, the rate of loss of mass is $kVc(t)$.



$$[q] = L^3/T$$

$$[c] = M/L^3$$

$$[V] = L^3$$

Dimension matrix $\to$

$$\begin{array}{c|c} & \begin{matrix} V & q & k & c_i & c_0 \end{matrix} \\ \begin{matrix} M \\ L \\ T \end{matrix} & \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ -3 & 3 & 0 & -3 & -3 \\ 0 & -1 & -1 & 0 & 0 \end{bmatrix} \end{array}$$

a) Write an ODE expressing mass balance:

$$\frac{d}{dt}(Vc(t)) = \underbrace{c_i q}_{\text{mass arrival rate}} - \underbrace{(qc(t) + Vkc(t))}_{\text{loss rate}}$$

Now, rewrite this as an ODE for $c'(t)$ and include any relevant initial conditions.

$$c'(t) = \frac{c_i q}{V} - \frac{qc(t)}{V} - kc(t) = -kc(t) - \frac{q}{V}(c - c_i)$$

IC = Initial condition $c(0) = c_0$ = initial concentration

b) Rewrite this ODE using general non-dimensionalization. $\bar{t} = \frac{t}{t_c}$ and $\bar{c} = \frac{c}{c_c}$. + IC

$$\bar{t} = \frac{t}{t_c} \to t = \bar{t}\, t_c$$

$$\bar{c} = \frac{c}{c_c} \Rightarrow c = \bar{c}\, c_c \to c' = \frac{c_c}{t_c}\frac{d\bar{c}}{d\bar{t}}$$

$$\xrightarrow{\text{Plugin}} \frac{c_c}{t_c}\frac{d\bar{c}}{d\bar{t}} = \frac{q}{V}(c_i - c_c\bar{c}) - kc_c\bar{c} \qquad \bar{c}(0) = \frac{c_0}{c_c}$$

c) Choose $t_c = k^{-1}$, $c_c = c_i$, rewrite the ODE for these choices of characteristic scale using the dimensionless parameters $\gamma := \frac{c_i}{c_0}$ and $\beta := \frac{kV}{q}$.

The ODE becomes

$$kc_i\frac{d\bar{c}}{d\bar{t}} = \frac{q}{V}(c_i - c_i\bar{c}) - kc_i\bar{c} \Rightarrow \frac{d\bar{c}}{d\bar{t}} = \frac{q}{kV}(1-\bar{c}) - \bar{c} = \frac{1}{\beta}(1-\bar{c}) - \bar{c}$$

$$\text{IC}: \bar{c}(0) = \gamma^{-1}$$

d) Find another timescale based on the parameters from the original problem. Repeat c) using this time scale and $c_c = c_i$.

Note that $[V/q] = T \Rightarrow$ Let $t_c = V/q$. This is the only other time scale.

ODE $\Rightarrow$ $$\frac{V}{q}c_i\frac{d\bar{c}}{d\bar{t}} = \frac{q}{V}(c_i - c_i\bar{c}) - kc_i\bar{c} = 1 - \bar{c} - \beta\bar{c} \quad \text{with IC} \quad \bar{c}(0) = \frac{1}{\gamma}$$

e) If we are in a regime where β is very small, which of the choices of timescale give an appropriate reformulation of the problem?

If $\beta \ll 1$, $\frac{1}{\beta}$ is very large. $\Rightarrow$ The second option is the best option.