

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 $Vc(t)$. Inside the tank the reactant decays at rate k , ie rate of loss of mass is $k \overbrace{Vc(t)}^{\text{mass inside}}$.



Write an ODE expressing mass balance: $\frac{d}{dt}(Vc(t)) = \underbrace{\text{mass arrival rate}} - \underbrace{\text{loss rate}}$

divide it by V :

Initial Condition is $c(0) = c_0$

How many params in model?

- Rewrite ODE & IC using general nondimensionalized $E = \frac{t}{t_c}$, $\varepsilon = \frac{c}{c_c}$ (leave t_c, c_c general for now).

A) Choose $t_c = k^{-1}$ and $c_c = c_i$, rewrite ODE & IC, expressing in terms of $\gamma := \frac{c_i}{c_0}$ and $\beta := \frac{kV}{q}$ (dimensionless params).

B) Instead change t_c to the other timescale derivable from original problem params. Keep c_c as before & rewrite ODE & IC

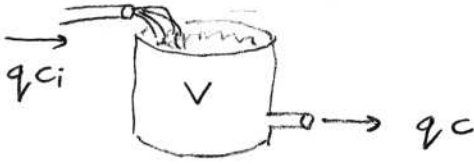
ie which ODE has sensible limit \uparrow as $\beta \rightarrow 0$?

C) if in reality $\beta \ll 1$ (what is the interpretation?) which of A or B is appropriate?

SOLUTIONS

... also see §1.2-2 in book → it's worked out in full.

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 $Vc(t)$. Inside the tank the reactant decays at rate k , i.e. rate of loss of mass is $kVc(t)$.



Write an ODE expressing mass balance:

Dimensions of all params:

M	V	q	k	c_i	c_0
L	+3	3		-3	-3
T		-1	-1		

$$\frac{d}{dt}(Vc(t)) = \overbrace{qc_i}^{\text{mass arrival rate}} - \overbrace{(qc + kVc)}^{\text{loss rate}}$$

divide it by V: $\dot{c} = \frac{q}{V}(c_i - c) - kc$

Initial Condition is $c(0) = c_0$

How many params in model? 5: V, q, k, c_0, c_i

Rewrite ODE & IC using general nondimensionalized $E = \frac{t}{t_c}, \bar{c} = \frac{c}{c_c}$ (leave t_c, c_c general for now).

Use the rules: $\begin{cases} c = c_c \bar{c} \\ \dot{c} = \frac{c_c}{t_c} \frac{d\bar{c}}{dE} \end{cases}$

sub. into ODE & IC

ODE: $\frac{c_c}{t_c} \frac{d\bar{c}}{dE} = \frac{q}{V}(c_i - c_c \bar{c}) - kc_c \bar{c}$

IC: $c_c \bar{c}(0) = c_0$

A) Choose $t_c = k^{-1}$ and $c_c = c_i$, rewrite ODE & IC, expressing in terms of $\gamma := \frac{c_i}{c_0}$ and $\beta := \frac{kV}{q}$ (dimensionless params).

sub. these into above:

$$c_i k \frac{d\bar{c}}{dE} = \frac{q}{V}(c_i - c_i \bar{c}) - kc_i \bar{c}$$

cancel $c_i, k \rightarrow \frac{d\bar{c}}{dE} = \frac{1}{\beta}(1 - \bar{c}) - \bar{c}$

IC: $\bar{c}(0) = \frac{1}{\gamma}$

B) Instead change t_c to the other timescale derivable from original problem params. Keep c_c as before & rewrite ODE & IC

look at dimensions matrix: $\left[\frac{V}{q} \right] = T$ is the only other timescale.

$$t_c = \frac{V}{q} \rightarrow c_i \frac{q}{V} \frac{d\bar{c}}{dE} = \frac{q}{V}(c_i - c_i \bar{c}) - kc_i \bar{c}$$

$$\Rightarrow \frac{d\bar{c}}{dE} = 1 - \bar{c} - \beta \bar{c} \quad \text{with IC } \bar{c}(0) = \frac{1}{\gamma}$$

ie which ODE has sensible limit as $\beta \rightarrow 0$?

C) if in reality $\beta \ll 1$ (what is the interpretation?) which of A or B is appropriate? By since in A, β diverges →