Nondimensionalization - Logistic Model

$$(1) \quad \frac{dP}{dT} = rP\left(1 - \frac{P}{K}\right) \qquad P(0) = P_0$$

where P is population (number N) at (dimensional) time T

$$[P] = N \qquad \text{number}$$

$$[T] = T \qquad \text{time}$$

One can deduce from (1) that

$$[r] = T^{-1} \qquad [K] = N \qquad [P_0] = N$$

Introduce dimensionless dependent and independent variables

$$(2) \quad p = P/P^* \qquad t = T/T^*$$

where P^*, T^* are to be determined and $[P^*] = N$, $[T^*] = T$

Using (2) in (1) yields

$$\frac{dp}{dt} = (rT^*)\, p\left(1 - p\frac{P^*}{K}\right) \qquad p(0) = P_0/P^*$$

Generally pick T^*, P^* s.t. resulting problem is as simple as possible.

$$(3) \quad \frac{dp}{dt} = p(1-p) \qquad p(0) = \alpha$$

where $\alpha = P_0/K$ using the choice

$$T^* = r^{-1} \qquad P^* = K$$

Advantages

(1) Dimensionless model has fewer parameters

(2) Sometimes small parameters exposed to aid in approximation schemes

Note:

(1) The choice of T^*, P^* are not unique. For example, the choice

$$T^* = 2r^{-1} \qquad P^* = P_0$$

would have resulted in

$$\frac{dp}{dt} = 2p(1 - \beta p) \qquad p(0) = 1$$

where $\beta = P_0/K$.

In our case the solution is relatively simple

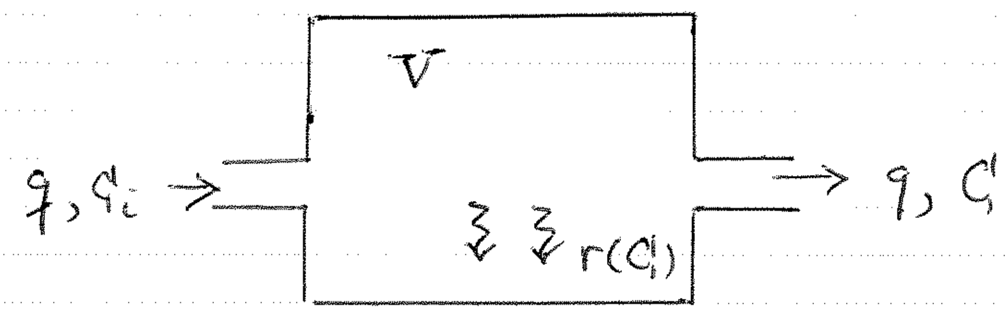
$$p(t) = \frac{\alpha}{\alpha + (1-\alpha)e^{-t}}$$

Continuously Stirred Tank Reactor (CSTR)

Chemical enters solvent filled tank of volume V at constant rate q with concentration c_i.

Tank contents are rapidly stirred so intratank concentration C is different than c_i in general.

Solvent reacts with reactant. Reactant disappears at rate $r(c)$.



Here

$$[V] = L^3$$

$$[c] = ML^{-3}$$

$$[q] = L^3 T^{-1} \quad \text{volume/time}$$

$$[r] = ML^{-3} T^{-1} \quad \text{mass/volume/time}$$

The latter <u>defines</u> what we mean by r.

<u>Note</u>: rate r is a function $r(c)$ of c

At any given (dimensional) time T

$V C_1$ = total mass of reactant in tank.

Thus, conservation of mass implies

$$\frac{d}{dT}(V C_1) = \underbrace{q C_i}_{\text{in}} - \underbrace{q C_1}_{\text{out}} - \underbrace{V r(C_1)}_{\text{reaction}}$$

Depending on the reactant $r(C_1)$ has different forms using <u>Law of Mass Action</u>

$$r(C_1) = k C_1 \qquad r(C_1) = \frac{k_1 C_1}{k_2 + C_1}$$

Using the former (as an assumption)

$$\boxed{\begin{aligned} \frac{dC_1}{dT} &= \frac{q}{V}(C_i - C_1) - k C_1 \\ C_1(0) &= C_0 \quad \text{(initial tank)} \end{aligned}}$$

is a model for C_1 at time T

Depends on many parameters

$q \quad V \quad C_i \quad k \quad C_0$

Nondimensionalization - CSTR model

$$(1) \quad \frac{dC'}{dT} = \frac{q}{V}(C'_i - C') - kC' \qquad C'(0) = C'_0$$

Introduce dimensionless variables

$$c = C'/C'^* \qquad [C^*] = ML^{-3}$$

$$t = T/T^* \qquad [T^*] = T$$

Yields

$$(2) \quad \frac{dc}{dt} = \frac{qT^*}{V}\left(\frac{C_i}{C^*} - c\right) - kT^*c \qquad c(0) = \frac{C_0}{C'^*}$$

There are many ways to choose C'^* and T^*.

Two obvious choices for C'^* are $C'^* = C_i, C_0$.

CHOICE ONE $\quad \boxed{C'^* = C'_i\ , \quad \frac{qT^*}{V} = 1}$

$$(3) \quad \frac{dc}{dt} = (1-c) - \beta c \qquad c(0) = \gamma$$

where

$$\beta = \frac{kV}{q} \qquad \gamma = C'_0 / C'_i$$

CHOICE TWO $\quad c^* = c_i \quad k\,T^* = 1$

$$(4) \qquad \frac{dc}{dt} = \frac{1}{\beta}(1-c) - c \qquad c(0) = \gamma$$

where β, γ are as defined before.

Slow Reaction Rate $\quad \beta \ll 1$

$\beta \ll 1$ dimensionless

$k \ll \frac{q}{V}$ dimensional equivalent

Thus $\beta \ll 1$ means the reaction rate k is small relative to the flow rate qV^{-1}.

$\beta \to 0^+$ approximation in CHOICE ONE

$c(t) \cong 1 + (\gamma - 1)e^{-t}$ OK

$\beta \to 0^+$ approximation in CHOICE TWO

$c(t) \cong 1$ X doesn't satisfy I.C.

Thus CHOICE ONE appears to be advantagous wrt approximations

There is no apriori way to systematically choose a "best" nondimensionalization.

CHOICE THREE (Not in text!)

$$\frac{dc}{dt} = \frac{qT^*}{V}\left(\frac{C_i}{C^*} - c\right) - kT^*c$$

$$\frac{dc}{dt} = \left(\frac{qT^*C_i}{VC^*}\right) - \left(\frac{qT^*}{V} + kT^*\right) c$$

choose C^* to make this one

choose T^* to make this one

Conclude (1-parameter model !!)

$$\boxed{\frac{dc}{dt} = 1 - c \qquad c(0) = \alpha}$$

where

$$T^* = \left(k + \frac{q}{V}\right)^{-1}$$

$$C^* = \frac{C_i q}{q + kV}$$

and $\alpha = C_0/C^*$

Clearly this less obvious choice results in the simplest dimensionless model