Aalto University

A continuously stirred isothermal reactor (I)

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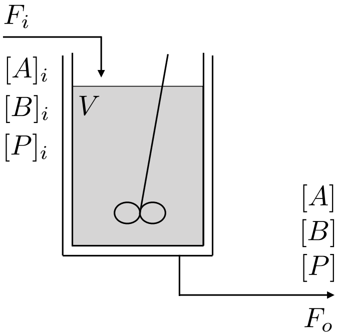
A continuously stirred isothermal reactor

Consider two chemical species A and B in a solvent feed entering a chemical reactor



Liquid-phase chemical reactor

$\rightsquigarrow$ Volume $V(t)$

Temperature is constant

$\rightsquigarrow$ $T(t) = \text{constant}$

The two species react to form a third species, the product component P ($A + 2B \longrightarrow P$)

We are interested in the reactor concentrations, as a function of time

A continuously stirred isothermal reactor (cont.)

Total mass balance

$$\underbrace{\frac{\mathrm{d}M(t)}{\mathrm{d}t}}_{\text{(mass/time)}} = \underbrace{\frac{\mathrm{d}V(t)\rho_0(t)}{\mathrm{d}t}}_{\text{(volume } \times \text{ (mass/volume) / times)}}$$

$$= \underbrace{\rho_i(t)}_{\text{(mass/volume)}} \underbrace{F_i(t)}_{\text{(volume/time)}} - \underbrace{\rho_o(t)}_{\text{(mass/volume)}} \underbrace{F_o(t)}_{\text{(volume/time)}}$$

(Rate of accumulation of mass = rate of mass entering - rate of mass leaving)

Assume that density is not a function of concentration

$\rightsquigarrow$ Thus, not a function of time $\rho_o(t) = \rho_i(t) = \rho$

We have,

$$\rightsquigarrow \quad \frac{\mathrm{d}V(t)}{\mathrm{d}t} = F_i(t) - F_o(t)$$

A continuously stirred isothermal reactor (cont.)

Component mass balance

Let $[A]$, $[B]$ and $[P]$ be molar concentrations (moles/volume) of species A, B and P

- We assumed the stoichiometric equation $A + 2B \longrightarrow P$

We also assume that there is no component P in the feed ($[P]_i(t) = 0$)

We can write,

$$\frac{\mathrm{d}\,V(t)[A](t)}{\mathrm{d}t} = F_i(t)[A]_i(t) - F_o(t)[A]_o(t) + V(t)r_A$$
$$\frac{\mathrm{d}\,V(t)[B](t)}{\mathrm{d}t} = F_i(t)[B]_i(t) - F_o(t)[B]_o(t) + V(t)r_B$$
$$\frac{\mathrm{d}\,V(t)[P](t)}{\mathrm{d}t} = F_i(t)\cancel{[P]_i(t)} - F_o(t)[P]_o(t) + V(t)r_P$$

Quantities r_A, r_B and r_P, generation rates of components A, B and P per unit volume

- moles/(volume $\times$ time)

A continuously stirred isothermal reactor (cont.)

We can assume that the reaction rate per unit volume for component A is second order

- We can also assume that it depends on the composition of both A and B

$$r_A(t) = -k[A](t)[B](t), \quad \text{(rate of generation of } A\text{, per unit volume)}$$

- k is the reaction rate constant

The stoichiometric equation tells us that one mole of A reacts with two moles of B

- ... to produce one mole of P

We can thus write

$$r_B(t) = -2k[A](t)[B](t) \quad \text{(rate of generation of } B\text{, per unit volume)}$$

and

$$r_P(t) = k[A](t)[B](t) \quad \text{(rate of generation of } P\text{, per unit volume)}$$

A continuously stirred isothermal reactor (cont.)

Consider the mass balance for component A,

$$\frac{\mathrm{d}V(t)[A](t)}{\mathrm{d}t} = V(t)\frac{\mathrm{d}[A](t)}{\mathrm{d}t} + [A](t)\frac{\mathrm{d}V(t)}{\mathrm{d}t} = F_i(t)[A]_i(t) - V(t)\underbrace{k[A](t)[B](t)}_{-r_A}$$

$$\rightsquigarrow \frac{\mathrm{d}[A](t)}{\mathrm{d}t} = \frac{F_i(t)[A]_i(t) - F_o(t)[A](t) - Vk[A](t)[B](t)}{V} - \frac{[A](t)}{V}\frac{\mathrm{d}V(t)}{\mathrm{d}t}$$

From the total mass balance, we have that $\mathrm{d}[A](t)/\mathrm{d}t = F_i(t) - F_o(t)$, thus

$$\begin{aligned}\frac{\mathrm{d}[A](t)}{\mathrm{d}t} &= \frac{F_i(t)[A_i(t)]}{V} - \cancel{\frac{F_o(t)[A](t)}{V(t)}} - k[A](t)[B](t) - \frac{[A](t)}{V(t)}F_i(t) + \cancel{\frac{[A](t)}{V(t)}F_o(t)}\\ &= \frac{F_i(t)}{V(t)}\Big([A]_i(t) - [A](t)\Big) - k[A](t)[B](t)\end{aligned}$$

Similarly, for the other two components

$$\rightsquigarrow \quad \frac{\mathrm{d}[B](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}\Big([B]_i(t) - [B](t)\Big) - 2k[A](t)[B](t)$$

$$\rightsquigarrow \quad \frac{\mathrm{d}[P](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}\Big(\underbrace{[P]_i(t)}_{=0} - [P](t)\Big) + k[A](t)[B](t)$$

A continuously stirred isothermal reactor (cont.)

Altogether, we have

$$\begin{aligned}
\frac{\mathrm{d}[A](t)}{\mathrm{d}t} &= \frac{F_i(t)}{V(t)}\Big([A]_i(t) - [A](t)\Big) - k[A](t)[B](t) \\
\frac{\mathrm{d}[B](t)}{\mathrm{d}t} &= \frac{F_i(t)}{V(t)}\Big([B]_i(t) - [B](t)\Big) - 2k[A](t)[B](t) \\
\frac{\mathrm{d}[P](t)}{\mathrm{d}t} &= -\frac{F_i(t)}{V(t)}[P](t) + k[A](t)[B](t) \\
\frac{\mathrm{d}V(t)}{\mathrm{d}t} &= F_i(t) - F_o(t)
\end{aligned}$$

The state equation of the model consists of four first-order differential equations

- $\rightsquigarrow$ Four state variables $V(t)$, $[A](t)$, $[B](t)$ and $[P](t)$

Four initial conditions (at $t = 0$) needed for determining the solution

- $\rightsquigarrow$ $V(0)$, $[A](0)$, $[B](0)$ and $[P](0)$

The system model also consists of four (five) input variables

- $\rightsquigarrow$ $F_i(t)$, $F(t)$, $[A]_i(t)$, and $[B]_i(t)$ (and $[P]_i(t)$)

A continuously stirred isothermal reactor (cont.)

$$\begin{bmatrix} \dot{V}(t) \\ [\dot{A}](t) \\ [\dot{B}](t) \\ [\dot{P}](t) \end{bmatrix} = \begin{bmatrix} F_i(t) - F_o(t) \\ \frac{F_i(t)}{V(t)}\Big([A]_i(t) - [A](t)\Big) - k[A](t)[B](t) \\ \frac{F_i(t)}{V(t)}\Big([B]_i(t) - [B](t)\Big) - 2k[A](t)[B](t) \\ -\frac{F_i(t)}{V(t)}[P](t) + k[A](t)[B](t) \end{bmatrix}$$

Note that the model has a single parameter k, which we assumed to be time-invariant

$\rightsquigarrow$ $k \neq k(t)$

A continuously stirred isothermal reactor (cont.)

Let

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ x_4(t) \end{bmatrix} = \begin{bmatrix} V(t) \\ [A](t) \\ [B](t) \\ [P](t) \end{bmatrix}, \quad u(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \\ u_4(t) \end{bmatrix} \begin{bmatrix} F_(t) \\ F_o(t) \\ [A]_i(t) \\ [B]_i(t) \end{bmatrix}, \quad \theta = [\theta_1] = [k]$$

We can write,

$$\underbrace{\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \\ \dot{x}_4(t) \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} f_1(x(t), u(t)|\theta) \\ f_2(x(t), u(t)|\theta) \\ f_3(x(t), u(t)|\theta) \\ f_4(x(t), u(t)|\theta) \end{bmatrix}}_{f(x,u|\theta)} = \begin{bmatrix} u_1(t) - u_2(t) \\ \frac{u_1(t)}{x_1(t)}\big(u_3(t) - x_2(t)\big) - kx_2(t)x_3(t) \\ \frac{u_1(t)}{x_1(t)}\big(u_4(t) - x_3(t)\big) - 2kx_2(t)x_3(t) \\ -\frac{u_1(t)}{x_1(t)x_4(t)} + kx_2(t)x_3(t) \end{bmatrix}$$

A continuously stirred isothermal reactor (cont.)

Let $x'(t) = [x(t) - x_{SS}(t)]$, $u'(t) = [u(t) - u_{SS}(t)]$, for some steady-state (x_{SS}, u_{SS})

We can write the linearised model, $\dot{x}'(t) = Ax'(t) + Bu'(t)$

$$A = \begin{bmatrix} \frac{\partial f_1(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_2(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_3(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_4(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \end{bmatrix}$$

$$B = \begin{bmatrix} \frac{\partial f_1(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_2(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_3(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_4(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \end{bmatrix}$$

A continuously stirred isothermal reactor (cont.)

$$A = \begin{bmatrix} 0 & 0 & 0 & \\ -\left.\frac{u_1(u_3 - x_2)}{x_1^2}\right|_{SS} & \left.\frac{u_1 x_3 k}{x_1}\right|_{SS} & -kx_2\Big|_{SS} & 0 \\ -\left.\frac{u_1(u_4 - x_2)}{x_1^2}\right|_{SS} & 2x_3 k\Big|_{SS} & \left.\frac{u_1 x_2 k}{x_1}\right|_{SS} & 0 \\ \left.\frac{u_1 x_4}{x_1^2}\right|_{SS} & k & x_2 k\Big|_{SS} & -\left.\frac{u_1}{x_1}\right|_{SS} \end{bmatrix}$$

$$B = \begin{bmatrix} 1 & -1 & 0 & \\ \left.\frac{u_3 - x_2}{x_1}\right|_{SS} & 0 & \left.\frac{u_1}{x_1}\right|_{SS} & 0 \\ \left.\frac{u_4 - x_3}{x_1}\right|_{SS} & 0 & 0 & \left.\frac{u_1}{x_1}\right|_{SS} \\ -\left.\frac{x_4}{x_1}\right|_{SS} & 0 & 0 & 0 \end{bmatrix}$$

For some fixed point (x_{SS}, u_{SS})