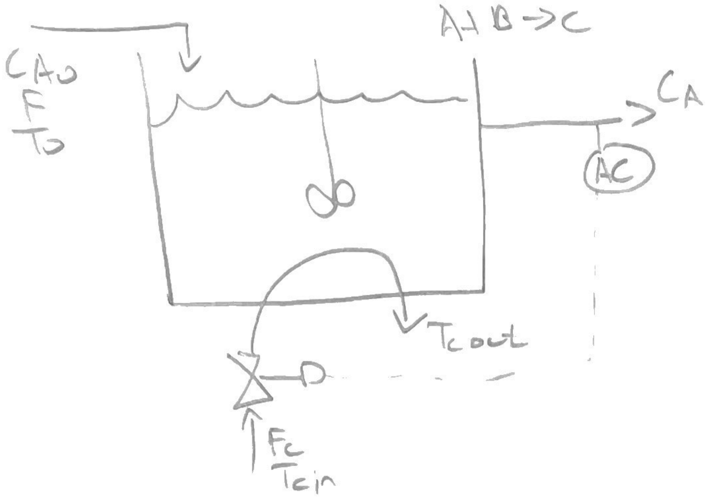
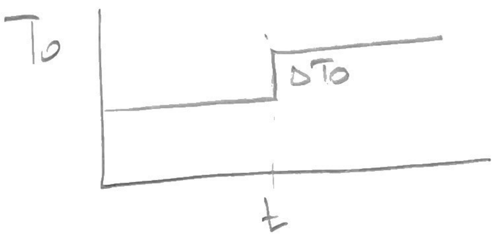
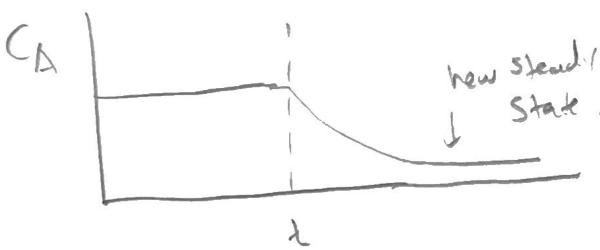
Process Dynamics - Ch. 3

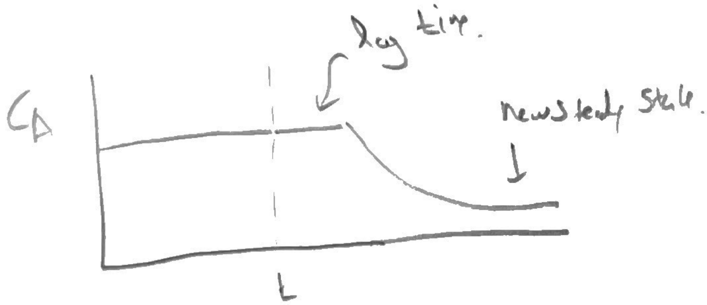
- Non-isothermal CSTR



Initially, $C_A = C_{A\,init}$ and the system is at steady state.
What happens to C_A if there is a step change in T_0?

- 





- T is also changing with time.

What is $C_A(t)$?

How long does it take for C_A to reach a new steady state?

What variables are important?

Mass, Component, & Energy Balance

$$\frac{d(\rho V)}{dt} = \rho_{in} F_{in} - \rho_{out} F_{out}$$

F: volumetric flow rate

ρ: density

Component Material

(mol/vol) (mol/vol·time)

molar: $$V \frac{dC_A}{dt} = F_{in} C_{A\,in} - F_{out} C_{A\,out} + V R_A$$

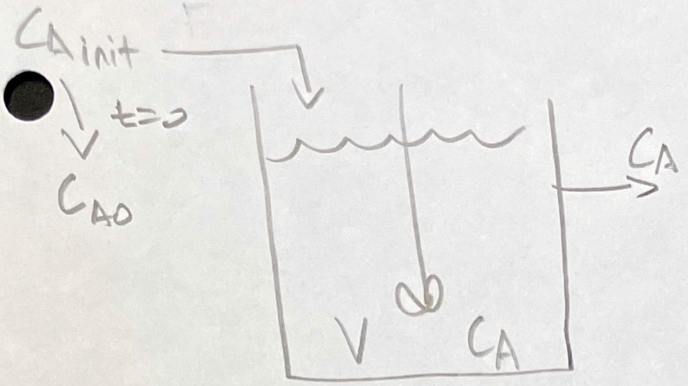
mass: $$MW_A V \frac{dC_A}{dt} = MW_A F_{in} C_{A\,in} - MW_A F_{out} C_{A\,out} + MW_A V R_A$$

Energy

$$\rho V c_p \frac{dT}{dt} = F_{in} \rho_{in} c_{p\,in} T_{in} - F_{out} \rho_{out} c_{p\,out} T_{out} + Q - W$$

(ignores potential & kinetic)

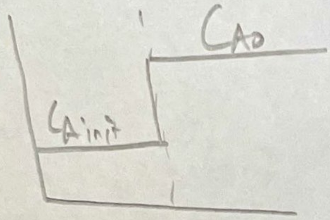
Mixing tank



F, ρ constant

For a mixing tank with constant flowrate F + liquid density ρ calculate $C_A(t)$ for a step change in $C_{A\,init}$.

Inlet Concentration



Component Balance.

$$V\frac{dC_A}{dt} = FC_{A0} - FC_A \qquad \text{for } t>0$$

Rearrange:

$$\frac{dC_A}{dt} + \frac{F}{V}C_A = \frac{F}{V}C_{A0} \qquad \text{define } V/F = \tau$$

$$\frac{dC_A}{dt} + \frac{1}{\tau}C_A = \frac{1}{\tau}C_{A0}$$

Use an integrating factor:

Multiply equation by $e^{t/\tau}$

$$e^{t/\tau}\frac{dC_A}{dt} + e^{t/\tau}\frac{1}{\tau}C_A = e^{t/\tau}\frac{1}{\tau}C_{A0}$$

$$\frac{d}{dt}\left(e^{t/\tau}C_A\right) = e^{t/\tau}\frac{1}{\tau}C_{A0}$$

$$e^{t/\tau}C_A = \int e^{t/\tau}\frac{1}{\tau}C_{A0}\,dt \quad + I$$

$$e^{t/\tau}C_A = e^{t/\tau}C_{A0} + I$$

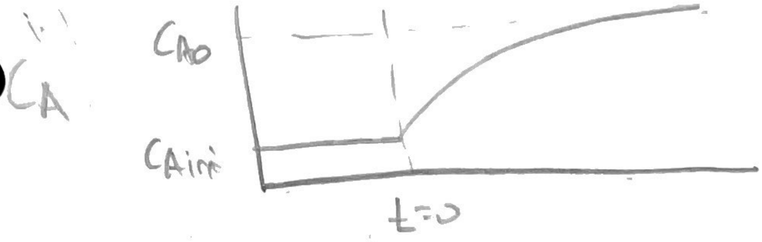
$$C_A = C_{A0} + I e^{-t/\tau} \qquad \text{for } t \geq 0$$

We need an initial condition for C_A

at $t=0$, $C_A = C_{Ainit}$

$$C_A(t=0) = C_{A0} + I \quad \Rightarrow \quad I = C_{Ainit} - C_{A0}$$

$$C_A = C_{A0} + (C_{Ainit} - C_{A0})e^{-t/\tau}$$

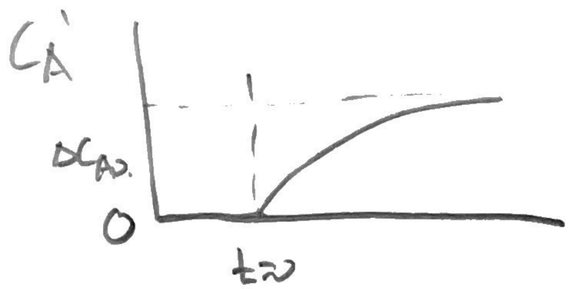


time	% to ss
0	0
τ	63%
2τ	86%
3τ	95%

at $t=3\tau$, system is at new ss

$$\underbrace{C_A - C_{Ainit}}_{C_A'} = \underbrace{C_{A0} - C_{Ainit}}_{\Delta C_{A0}} + \underbrace{(C_{Ainit} - C_{A0})}_{-\Delta C_{A0}} e^{-t/\tau}$$

$$C_A' = \Delta C_{A0}\left(1 - e^{-t/\tau}\right)$$



Integrating factor method:

$$\frac{dC_A}{dt} + \frac{1}{\tau} C_A = K\,F_{(t)}$$

Multiply by $e^{t/\tau}$; τ will depend on the specific problem

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Stirred chemical Reactor (Ex 3.2)

$A \xrightarrow{k} B$

F constant

$$(t>0) \qquad V\frac{dC_A}{dt} = F C_{A0} - F C_A - kVC_A$$

$$V\frac{dC_A}{dt} + FC_A + kVC_A = FC_{A0}$$

$$\frac{dC_A}{dt} + \underbrace{\left(\frac{F+kV}{V}\right)}_{1/\tau} C_A = \frac{F}{V} C_{A0}$$

$$\frac{dC_A}{dt} + 1/\tau\, C_A = F/V\, C_{A0} \qquad (t \geq 0)$$

$$\frac{dC_{As}}{dt} + 1/\tau\, C_{As} = F/V\, C_{A\,init} \qquad (t \leq 0)$$

Subtract Equations

$$C_A' = C_A - C_{As}$$

$$\Delta C_{A0} = C_{A0} - C_{Ainit}$$

$$\frac{dC_A'}{dt} + \frac{1}{\tau} C_A' = \frac{F}{V} \Delta C_{A0}$$

Solve using integrating factors

$$\left(\frac{dC_A'}{dt} + \frac{1}{\tau} C_A' \right) e^{t/\tau} = e^{t/\tau} F/V \, \Delta C_{A0}$$

$$\frac{d}{dt}\left(e^{t/\tau} C_A' \right) = e^{t/\tau} F/V \, \Delta C_{A0}$$

$$e^{t/\tau} C_A' = \int e^{t/\tau} F/V \, \Delta C_{A0} \, dt + I$$

$$e^{t/\tau} C_A' = \frac{F\tau}{V} \Delta C_{A0} e^{t/\tau} + I$$

$$C_A' = \frac{F\tau}{V} \Delta C_{A0} + I e^{-t/\tau}$$

at $t=0$, $C_A' = 0$. $\Rightarrow I = -\frac{F\tau}{V} \Delta C_{A0}$

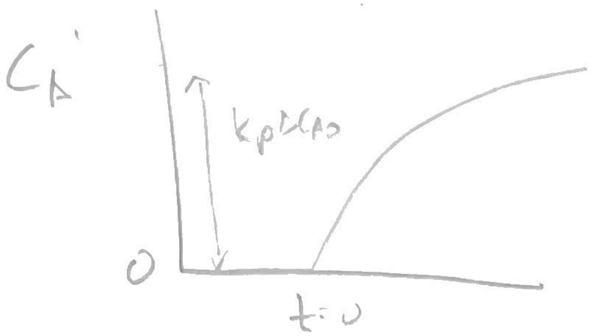
$$\underline{C_A' = \frac{F\tau}{V} \Delta C_{A0} \left(1 - e^{-t/\tau} \right)}$$

$$\tau = \frac{V}{F + kV}$$

as $t \to \infty$, $C_A' \to \frac{F\tau}{V} \Delta C_{A0} = \underbrace{\frac{F}{F+kV}}_{K_p} \Delta C_{A0}$

$$\underline{C_A' = K_p \Delta C_{A0} \left(1 - e^{-t/\tau} \right)}$$

$$C_{As} = K_p C_{Ainit}$$



Second-order differential equation

Component balance for each reactor

$$V_1 \frac{dC_{A1}}{dt} = F(C_{A0} - C_{A1}) - V_1 k C_{A1}$$

$$V_2 \frac{dC_{A2}}{dt} = F(C_{A1} - C_{A2}) - V_2 k C_{A2}$$

This is a second order problem

<u>for $t<0$</u>

$$V_1 \frac{dC_{A1s}}{dt} = F(C_{A\,init} - C_{A1s}) - V_1 k C_{A1}$$

$$V_2 \frac{dC_{A2}}{dt} = F(C_{A1s} - C_{A2s}) - V_2 k C_{A2s}$$

Subtract Equations

$$V_1 \frac{dC_{A1}'}{dt} = F(\Delta C_{A0} - C_{A1}') - V_1 k C_{A1}'$$

$$V_2 \frac{dC_{A2}'}{dt} = F(C_{A1}' - C_{A2}') - V_2 k C_{A2}'$$

Solve for C_{A1}':

$$\frac{dC_{A1}'}{dt} + \frac{F + kV_1}{V_1} C_{A1}' = \frac{F}{V_1} \Delta C_{A0} \qquad \tau_1 = \frac{V_1}{F + kV_1}$$

Solve as prior problem

$$C_{A1S}' = K_{p1} \Delta C_{A0} (1 - e^{-t/\tau}) \qquad K_{p1} = \frac{F}{F + kV_1}$$

Solve for C_{A2}':

$$V_2 \frac{dC_{A2}'}{dt} = F\left(K_{p1} \Delta C_{A0} (1 - e^{-t/\tau}) - C_{A2}' \right) - V_2 k C_{A2}'$$

$$\frac{dC_{A2}'}{dt} + \underbrace{\frac{F + V_2 k}{V_2}}_{1/\tau_2} C_{A2}' = \frac{F K_{p1} \Delta C_{A0}}{V_2} (1 - e^{-t/\tau})$$

Set $V_1 = V_2$

$$\tau_1 = \frac{V_1}{F+kV_1} = \tau_2 = \frac{V_2}{F+kV_2} = \tau$$

$$K_{p1} = \frac{F}{F+kV_1} = \frac{F}{F+kV_2} = K_{p2}$$

$$\frac{dC_{A2}'}{dt} + \frac{1}{\tau} C_{A2}' = \frac{F K_p \Delta C_{A0}}{V}\left(1 - e^{-t/\tau}\right)$$

Solve using integrating factor $e^{t/\tau}$

$$\frac{d}{dt}\left(C_{A2}' e^{t/\tau}\right) = \frac{F K_p}{V} \Delta C_{A0} \left(e^{t/\tau} - 1\right)$$

$$C_{A2}' e^{t/\tau} = \frac{F K_p \Delta C_{A0}}{V}\left(\tau e^{t/\tau} - t\right) + I$$

at $t=0$, $C_{A2}' = 0$

$$I = -\frac{F K_p \Delta C_{A0}}{V} \tau$$

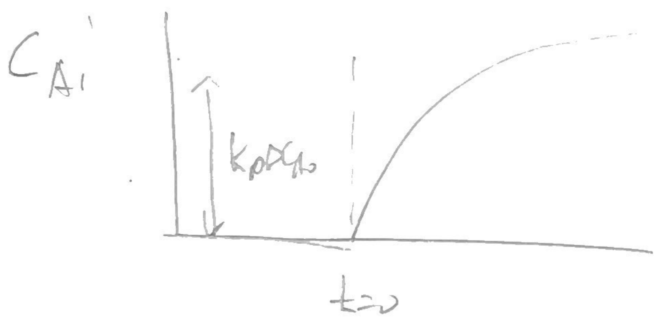
$$C_{A2}' e^{t/\tau} = \frac{F K_p \Delta C_{A0}}{V}\left(\tau e^{t/\tau} - t\right) - \frac{F K_p \Delta C_{A0}}{V} \tau$$

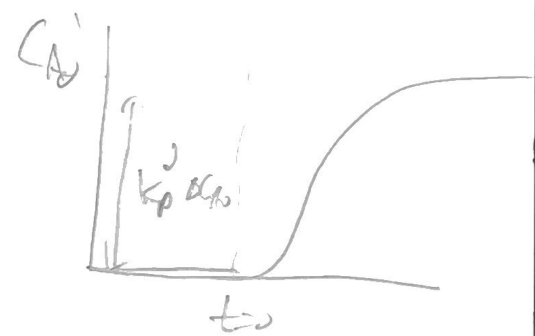
$$C_{A2}' e^{t/\tau} = \frac{F K_p \Delta C_{A0}}{V} \tau \left(e^{t/\tau} - 1\right) - \frac{F K_p \Delta C_{A0}}{V} t$$

$$C_{A_d}' = \frac{F K_p \Delta C_{A_0}}{V}\tau\left(1 - e^{-t/\tau}\right) - \frac{F K_p \Delta C_{A_0}}{V} t e^{-t/\tau}$$

$$\frac{F K_p}{V}\tau = \frac{F}{V}\cdot\frac{V}{F+kV}\cdot K_p = K_p^2$$

$$C_{A_d}' = K_p^2 \Delta C_{A_0}\left(1 - e^{-t/\tau}\right) - K_p^2 \Delta C_{A_0} \frac{t}{\tau} e^{-t/\tau}$$





We have an approach to analyze process dynamics

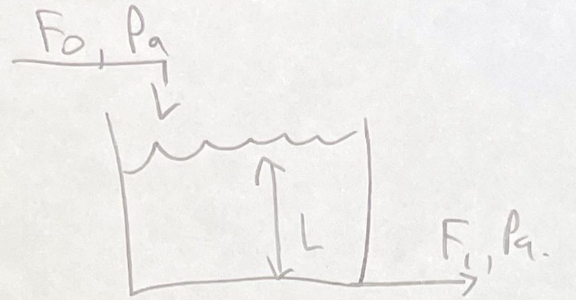
- applies to 1^{st}, 2^{nd}, higher order systems
- only applicable to linear systems

  e.g. $V\frac{dC_A}{dt} = -VKC_A^2$ is non-linear

  we will use Taylor expansion to deal with this

- only applies to step change, not pulse or gradual change in C_{A0}

Example of a non-linear problem



$$\rho A \frac{dL}{dt} = \rho F_0 - \rho F_1$$

Constitutive equation: $F_1 = k_{F_1} L^{1/2}$

$$\rho A \frac{dL}{dt} = \rho F_0 - \underbrace{\rho k_{F_1} L^{1/2}}$$

non-linear. cannot use integrating factor

Taylor Expansion: $f(L) \approx f(L=L_s) + \left.\frac{df}{dL}\right|_{L=L_s} (L - L_s)$

$$L^{1/2} \approx L_s^{1/2} + \tfrac{1}{2} L_s^{-1/2} (L - L_s).$$

$$\rho A \frac{dL}{dt} = \rho F_0 - \rho k_{F_1} \left(L_s^{1/2} + \tfrac{1}{2} L_s^{-1/2} L - \tfrac{1}{2} L_s^{1/2} \right)$$

Use deviation vars.

$$\rho A \frac{dL'}{dt} = \rho \Delta F_0 - \rho k_{F_1} \left(\tfrac{1}{2} L_s^{-1/2} L' \right)$$

$$\frac{dL'}{dt} + \underbrace{\frac{1}{2}\frac{k_{F_1} L_s^{-1/2}}{A}}_{1/\tau} L' = \frac{\Delta F_0}{A}$$

Solve as before.

$$L' = \frac{\tau \Delta F_0}{A}\left(1-e^{-t/\tau}\right)$$

$$\tau = \frac{2A}{k_{F_1} L_s^{-1/2}} \qquad K_p = \frac{2}{k_{F_1} L_s^{-1/2}}$$

Another Non-linear Problem

Reactor with $R_A = -kC_A^2$

$$V\frac{dC_A}{dt} = F(C_{A_0} - C_A] - \underbrace{kC_A^2}_{\text{non-linear}} V$$

$$C_A^2 \approx C_{A_s}^2 + 2C_{A_s}(C_A - C_{A_s}) + \dots$$

$$V\frac{dC_A}{dt} = F(C_{A_0} - C_A) - kV\left(C_{A_s}^2 + 2C_{A_s}C_A - 2C_{A_s}^2\right)$$

for $t<0$ $$V\frac{dC_{A_s}}{dt} = F(C_{A_{ini}} - C_{A_s}) - kV\left(C_{A_s}^2 + 2C_{A_s}^2 - 2C_{A_s}^2\right)$$

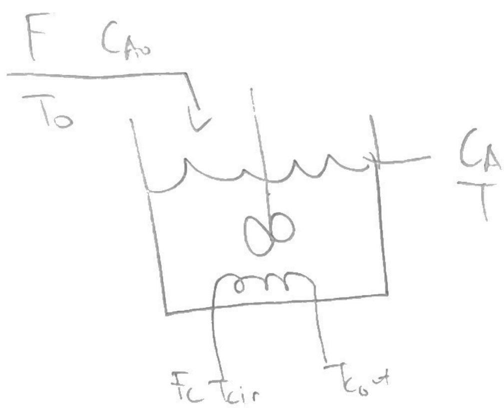
$$V\frac{dC_A'}{dt} = F(\Delta C_{A0} - C_A') - kV(2C_{As}C_A')$$

$$\frac{dC_A'}{dt} + \underbrace{\frac{F+2kVC_{As}}{V}}_{1/\tau} C_A' = \underbrace{\frac{F}{V}}_{k_p/\tau} \Delta C_{A0}$$

$$C_A' = k_p \Delta C_{A0}\left(1 - \exp(-t/\tau)\right)$$

$$\tau = \frac{V}{F+2kVC_{As}} \qquad k_p = \frac{F}{F+2kVC_{As}}$$

Non-isothermal reactor



$$V\frac{dC_A}{dt} = F(C_{A0} - C_A) - Vk_0e^{-E/RT}C_A$$

Energy

$$\rho V C_p \frac{dT}{dt} = F\rho C_p(T_0 - T) + U(T - T_c)$$
$$+ (-\Delta H_{rxn})Vk_0e^{-E/RT}C_A$$

Solve numerically See textbook or Matlab code in Canvas

Mixing tank example: what if there's a step chge in F instead of C_{A0}?

$$V\frac{dC_A}{dt} = F(C_{A0} - C_A)$$

$$V\frac{dC_A}{dt} = FC_{A0} - \underbrace{FC_A}_{\text{non-linear}}$$

$$FC_A \approx F_s C_{As} + F_s(C_A - C_{As}) + C_{As}(F - F_s)$$

$$V\frac{dC_A}{dt} = FC_{A0} - F_s C_{As} - F_s C_A + F_s C_{As} - FC_{As} + C_{As}F_s$$

Use deviation variable

$$V\frac{dC_A'}{dt} = \Delta F\, C_{A0} - F_s C_A' - \Delta F\, C_{As}$$

$$\frac{dC_A'}{dt} + \underbrace{\frac{F_s}{V}}_{1/\tau} C_A' = \underbrace{\frac{1}{V}(C_{A0} - C_{As})}_{K_p/\tau}\Delta F$$

$$C_A' = K_p(1 - e^{-t/\tau}), \quad \tau = \frac{V}{F_s}, \quad K_p = \frac{C_{A0} - C_{As}}{V}$$

If F and C_{A0} are both changing then we find the deviation for each and add them together