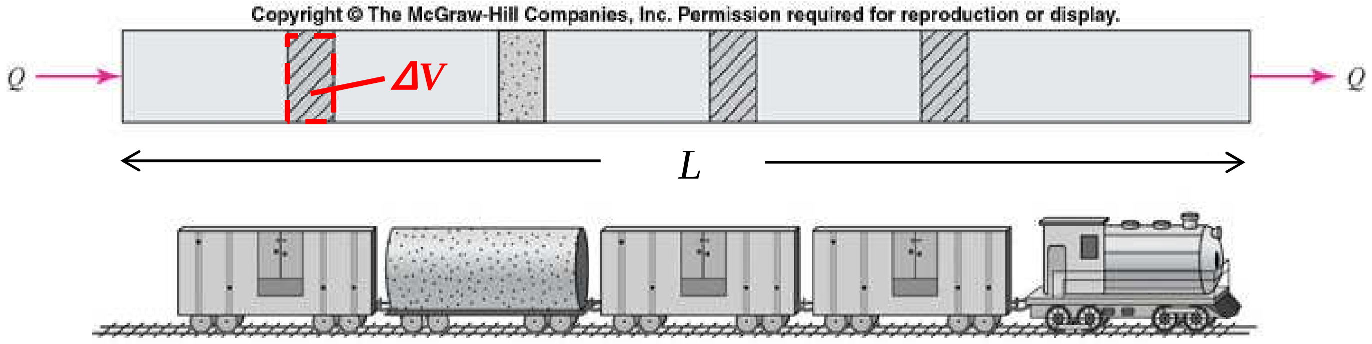
Reactors II

Today's lecture

- Reactor analysis using mass balance
  - Plug flow reactor
  - Completely mixed flow reactor

Reactor analysis – PFR, 1^{st} order reaction

- Plug-flow reactor (PFR)



V = reactor volume

1) define control volume:

the moving "plug": a very thin, homogeneous plate moving in the direction of flow

Reactor analysis – PFR, 1st order reaction

2) write a mass balance eq.:

$$\boxed{\frac{dM}{dt}} = \cancel{\frac{d(in)}{dt}} - \cancel{\frac{d(out)}{dt}} + \boxed{R}$$

$\nearrow$ $\Delta V \frac{dC}{dt}$

$\nwarrow$ $-kC\Delta V$ (1st order)

3) arrange the equation: $\frac{dC}{dt} = -kC$

integrating over $t=0$ to t_0 (= L/v_{flow} = V/Q):

$$\frac{C_{out}}{C_{in}} = e^{-kt_0}$$

→ same form as the batch reactor!

(why??)

Reactor analysis – PFR, 1st order reaction

- Examples of PFRs

Disinfection

Rivers and streams

Reactor analysis - PFR

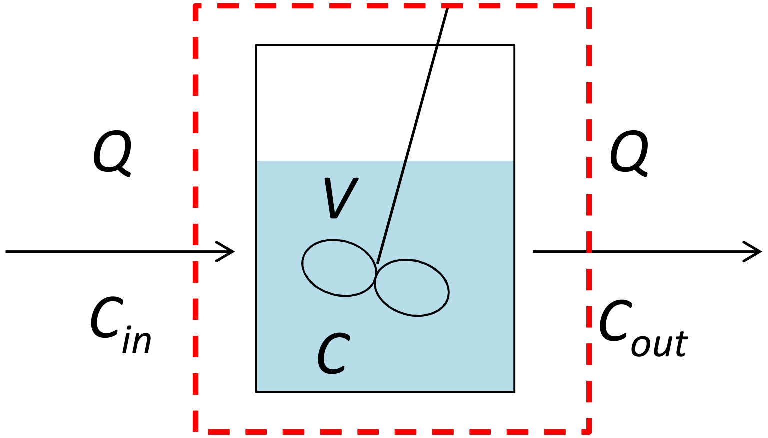
Q: In the U.S., a wastewater treatment plant must disinfect its effluent before discharging the wastewater to a stream. The wastewater contains 4.5 x 10^5 CFU/L of fecal coliform. The effluent standard for fecal coliform is 2 x 10^3 CFU/L. Assuming that the disinfection facility is a PFR, determine the length of pipe required if the velocity of the wastewater in the PFR is 0.75 m/s. Assume that the first-order reaction rate constant for destruction of the fecal coliforms is 0.23 min^{-1}.

Reactor analysis – CMFR, 1st order reaction

- Completely mixed flow reactor (CMFR) (continuous-flow stirred tank reactor, CSTR)

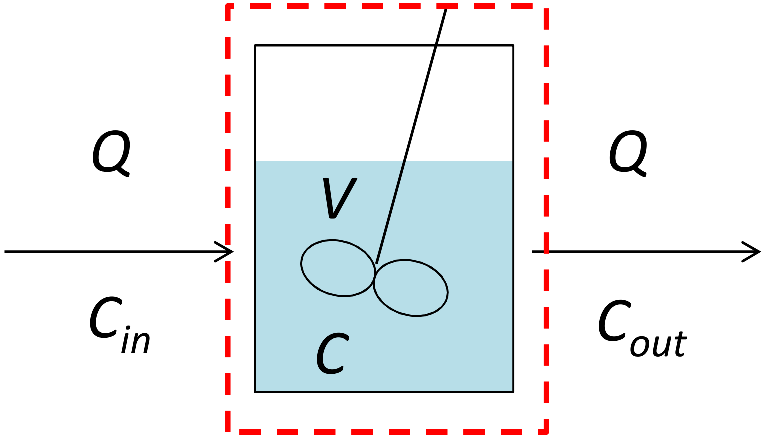
1) define control volume

2) write a mass balance eq.



$$\underbrace{\frac{dM}{dt}}_{V\frac{dC}{dt}} = \underbrace{\frac{d(in)}{dt}}_{Q\cdot C_{in}} - \underbrace{\frac{d(out)}{dt}}_{Q\cdot C_{out}} + \underbrace{R}_{-kCV\ (1^{st}\ \text{order})}$$

Reactor analysis – CMFR, 1st order reaction



Because of homogeneous mixing, $C = C_{out}$

$$V\frac{dC_{out}}{dt} = QC_{in} - QC_{out} - kC_{out}V$$

Reactor analysis – CMFR, 1st order reaction

3) arrange the equation:

$$V\frac{dC_{out}}{dt} = QC_{in} - QC_{out} - kC_{out}V$$

Special case I: No reaction, initial concentration = C_0

$$V\frac{dC_{out}}{dt} = QC_{in} - QC_{out} - \cancel{kC_{out}V}$$

$$\frac{dC_{out}}{dt} = \frac{1}{t_o}(C_{in} - C_{out}) \qquad (t_0 = V/Q)$$

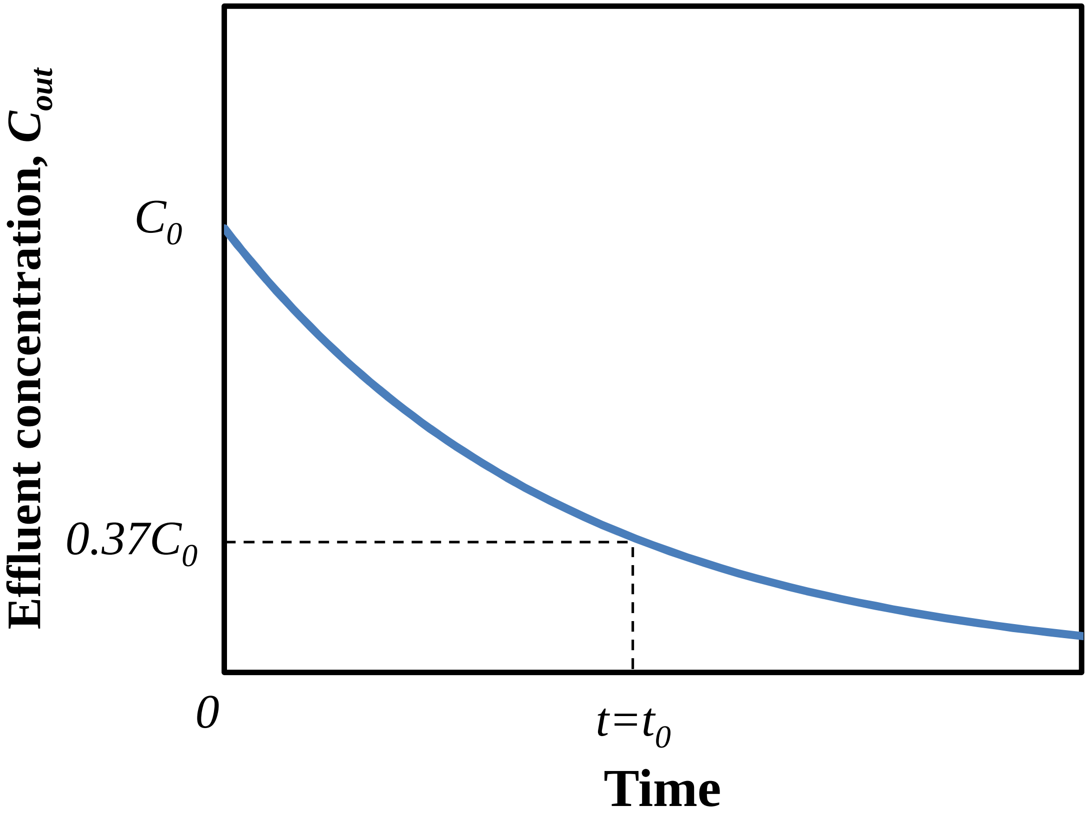
integrating over t=0 to t:

$$C_{out,t} = \boxed{C_o\left[exp\left(-\frac{t}{t_0}\right)\right]} + \boxed{C_{in}\left[1 - exp\left(-\frac{t}{t_0}\right)\right]}$$

Reactor analysis – CMFR, 1^{st} order reaction

when $C_{in} = 0$,

$$C_{out,t} = C_o\left[exp\left(-\frac{t}{t_0}\right)\right]$$



Reactor analysis – CMFR, 1st order reaction

$$V\frac{dC_{out}}{dt} = QC_{in} - QC_{out} - kC_{out}V$$

Special case II: Steady state

$$V\cancelto{}{\frac{dC_{out}}{dt}} = QC_{in} - QC_{out} - kC_{out}V$$

$$C_{out} = \frac{C_{in}}{1 + kt_0} \qquad (t_0 = V/Q)$$

→ influent concentration (C_{in}) is reduced in the effluent by a factor of ($1+kt_0$)

Reactor analysis – CMFR, 1st order reaction

- Examples of CMFRs

Biological wastewater treatment

Lake

Reactor analysis - CMFR

Q: Activated sludge is a key process for most wastewater treatment facilities. The process is often run as a CMFR. Assume a 400 m^3-sized CMFR for an activated sludge process receiving 2000 m^3/d of wastewater. If a terrorist dumped 10 kg of a non-biodegradable toxic chemical to the reactor, how long will it take for the toxic chemical concentration in the reactor to a safe level (1 mg/L)?

Reactor analysis - CMFR

Q: A chemical degrades in a steady-state CMFR according to first-order reaction kinetics. The upstream concentration of the chemical is 10 mg/L and the downstream concentration is 2 mg/L. Water is being treated at a rate of 29 m^3/min. The volume of the tank is 580 m^3. What is the rate of decay? What is the rate constant?

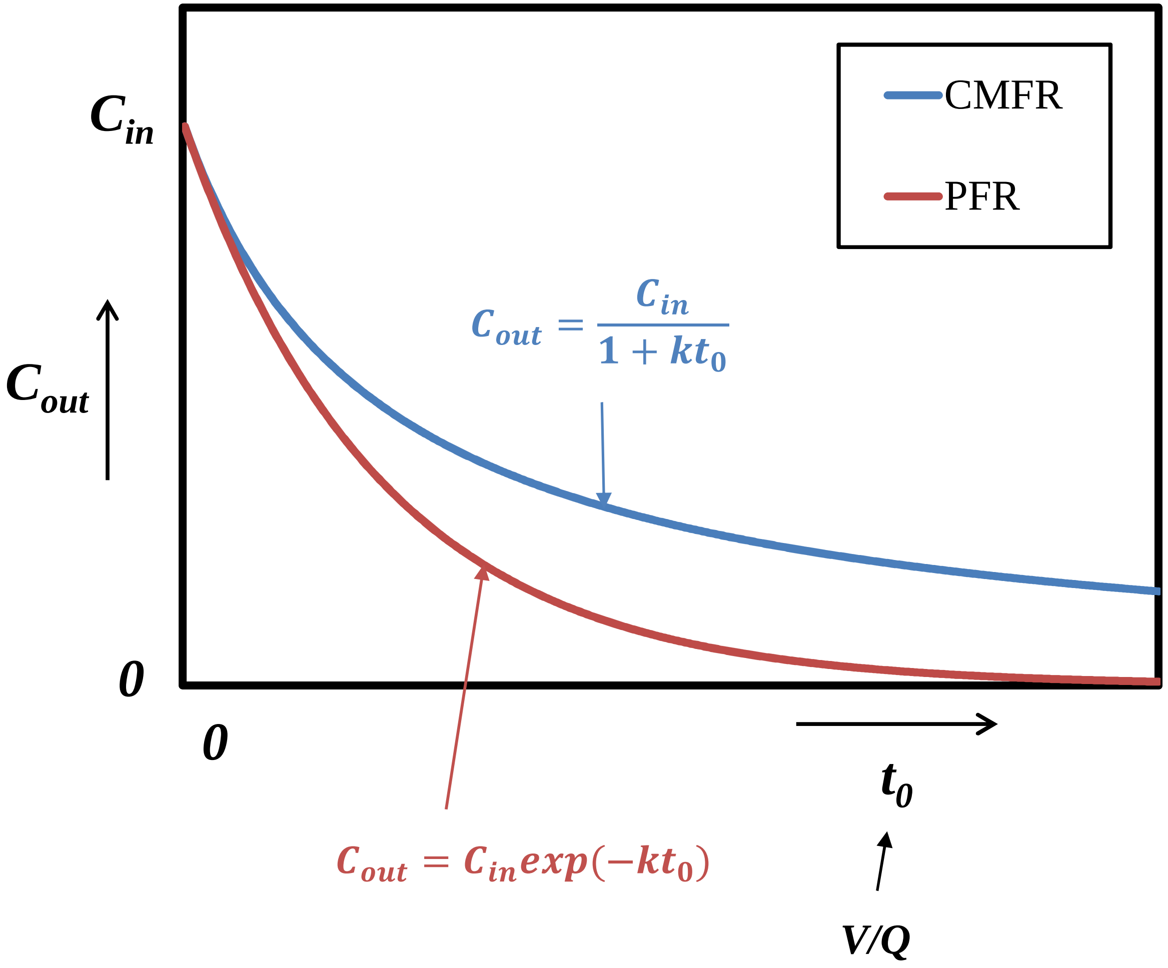
Retention time

- Retention time (detention time), t_0

  $$t_0 = V / Q$$

  - The average time the fluid particles spend in the reactor
  - PFR: the time that fluid particles spend in a reactor is the same (=t_0) for all particles
  - CMFR: the time that fluid particles spend in a reactor is different

PFR vs. CMFR



$$C_{out} = \frac{C_{in}}{1 + kt_0}$$

$$C_{out} = C_{in} exp(-kt_0)$$

- At the same t_0, PFR shows better performance
- Advantage of using CMFR: less sensitive to shock loads and toxic compounds

Reading assignment

- Textbook Ch4 p. 162-168

Reactor analysis - PFR

Slide#6 solution)

$$ln\frac{C_{out}}{C_{in}} = -kt_0 = -kL/v_{flow}$$

$$L = -\frac{v_{flow}}{k} \cdot ln\frac{C_{out}}{C_{in}} = -\frac{0.75\ m/s}{0.23\ min^{-1}} \times 60\ s/min \times ln\frac{2\times10^3\ CFU/mL}{4.5\times10^5\ CFU/mL}$$

$$= \mathbf{1060\ m}$$

Reactor analysis - CMFR

Slide#13 solution)

Non-biodegradable → no reaction

$$C_{out,t} = C_0 exp(-t/t_0)$$

$$t = -t_0 \cdot ln\frac{C_{out,t}}{C_0}$$

$$C_0 = \frac{10\ kg}{400\ m^3} \times 10^6\ mg/kg\ \times\ 10^{-3}\ m^3/L = 25\ mg/L$$

$$t_0 = \frac{V}{Q} = \frac{400\ m^3}{2000\ m^3/d} = 0.2\ d$$

$$t = -0.2\ d \cdot ln\frac{1\ mg/L}{25\ mg/L} = \mathbf{0.64\ day}$$

Reactor analysis - CMFR

Slide#14 solution)

$$C_{out} = \frac{C_{in}}{1+kt_0}$$

$$k = \frac{1}{t_0}\left(\frac{C_{in}}{C_{out}} - 1\right)$$

$$t_0 = \frac{580\ m^3}{29\ m^3/min} = 20\ min$$

$$k = \frac{1}{20\ min}\left(\frac{10\ mg/L}{2\ mg/L} - 1\right) = \mathbf{0.20\ min^{-1}}$$

rate of decay $= -r = -\left.\frac{dC}{dt}\right|_{reaction} = k \cdot C_{out}$

$$= (0.20\ min^{-1}) \cdot (2\ mg/L) = \mathbf{0.40\ mg/L - min}$$