Mass balance
Reactors I

Today's lecture

- Mass balance
- Mixing and steady state
- Reactor analysis using mass balance
  - Completely mixed batch reactor

Basic theory

- Conservation of matter: matter (atoms) can neither be created nor destroyed
  - * exception (not relevant to this class!): $E = mc^2$

Mass balances (materials balances)

Simple accounting of materials:

(Accumulation) = (Input) – (Output)

like in your bank account,

balance = deposit - withdrawal

Mass balance: Time as a factor

[(Accumulation) = (Input) – (Output) **] / (time)**

$$\frac{dM}{dt} = \frac{d(in)}{dt} - \frac{d(out)}{dt}$$

rate of accumulation	rate of input	rate of output

- Solving a mass balance problem:
  1) Define control volume (system boundary)
  2) Write a mass balance equation using time as a factor
  3) Arrange it to a useful form

Solving a mass balance problem

Q: Prof. Choi is filling his bathtub but he forgot to put the plug in. If the volume of water for a bath is 0.350 m^3 and the tap is flowing at 1.32 L/min, and the drain is running at 0.32 L/min, how long will it take to fill the tub to bath level? At the time when the tub is filled, how much water will be wasted?

Mass balance: substances in water

$$\frac{dM}{dt} = \frac{d(in)}{dt} - \frac{d(out)}{dt}$$

For substances homogeneously distributed in water or air, ***d(in)/dt*** and ***d(out)/dt*** can be calculated as:

$$\frac{Mass}{Time} = C \cdot Q = Mass\ flow\ rate$$

C = concentration **[M/L^3]**

Q = flow rate **[L^3/T]**

Accordingly,

$$\frac{dM}{dt} = C_{in} \cdot Q_{in} - C_{out} \cdot Q_{out}$$

Steady state

- $dM/dt = 0$
- No change in the amount of materials in the control volume, i.e., $M \neq f(t)$

  cf) transient state: $M = f(t)$

- The mass balance equation gets simpler! (No left hand side term)

Mass balance: including reactions

(Accumulation) = (Input) – (Output) + (Reaction)

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

R = rate of change in mass due to reaction [M/T]

= *rV* (*V*: volume)

reaction rate, $r = -kC^n$ [M/L^3/T] (*n*=reaction order)

for 1st order reaction, $r = -kC$

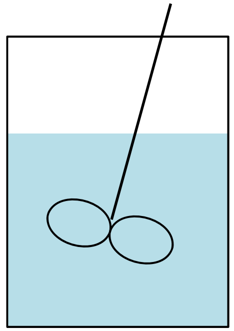
(most common in the environment)

Mass balance: including reactions

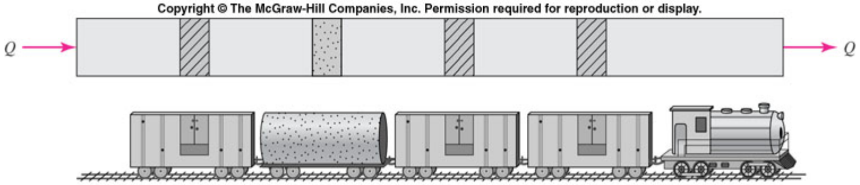
Q: A well-mixed sewage lagoon is receiving 430 m^3/d of untreated sewage. The lagoon has a surface area of 10 ha and a depth of 1.0 m. The pollutant concentration in the sewage discharging into the lagoon is 180 mg/L. The pollutants degrades in the lagoon according to first-order kinetics with a reaction rate constant of 0.70 d^{-1}. Assuming no other water losses or gains and that the lagoon is completely mixed, find the steady-state concentration of the pollutant in the lagoon effluent.

The state of mixing

- Ideal models for mixing
  - completely mixed systems: entire system is homogeneous



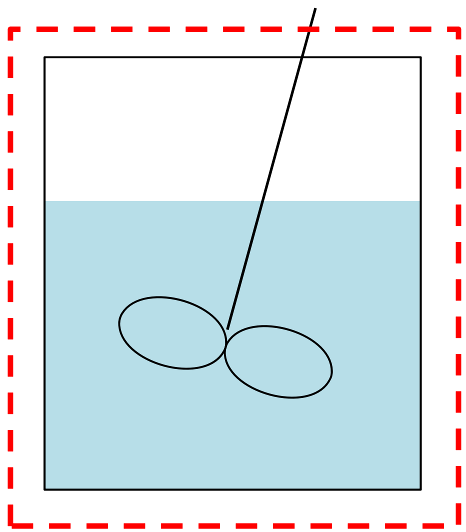
  - plug flow systems: no mixing in the direction of flow; homogeneous (completely mixed) in the direction perpendicular to the flow



(b)

Reactor analysis – CMBR, 1st order reaction

- **Completely mixed batch reactor (CMBR)**
  - Fill-and-draw type
  - No flow in or flow out



1) define control volume

2) write a mass balance eq.

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

$$V\frac{dC}{dt} \qquad -kCV$$

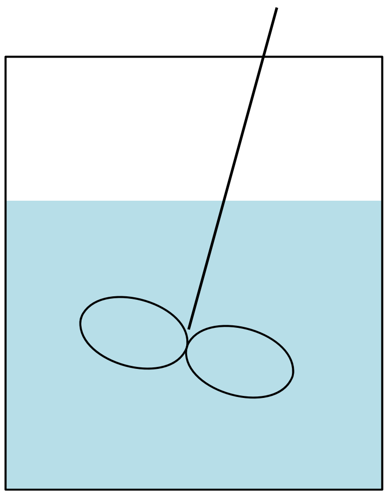
Reactor analysis - CMBR, 1^{st} order reaction

3) arrange the equation

$$\frac{dC}{dt} = -kC$$

integrating over $t=0$ to t_{final}:

$$\frac{C_{final}}{C_{initial}} = e^{-kt_{final}}$$



Reactor analysis - CMBR, 1^{st} order reaction

Q: A contaminated soil is to be treated in a completely mixed lagoon. To determine the time it will take to treat the soil, a laboratory completely mixed batch reactor is tested to gather the following data. Assuming a first-order reaction, estimate the rate constant, k, and determine the time to achieve 99% reduction in the original concentration.

Time (days)	Contaminant concentration (mg/kg)
1	280
16	132

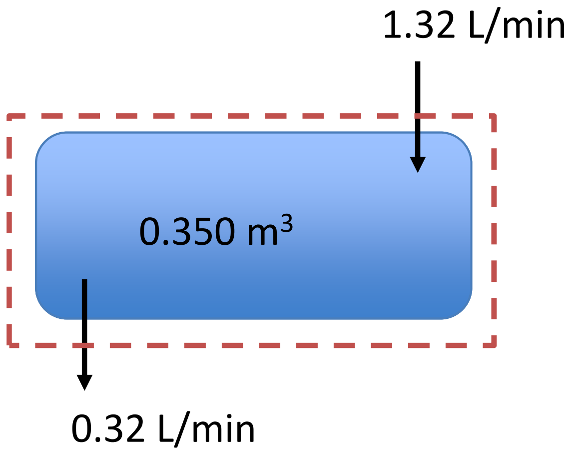
Reading assignment

- Textbook Ch4 p. 144-162

Solving a mass balance problem

Slide#6 solution)

i) Draw a schematic diagram, define CV



ii) Write a mass balance eq.

$$\frac{dM}{dt} = \frac{d(in)}{dt} - \frac{d(out)}{dt}$$

iii) Arrange the eq. to a useful form

As d(in)/dt and d(out)/dt are constant over time, dM/dt should be constant over time:

$$\frac{\Delta M}{\Delta t} = \frac{d(in)}{dt} - \frac{d(out)}{dt}$$

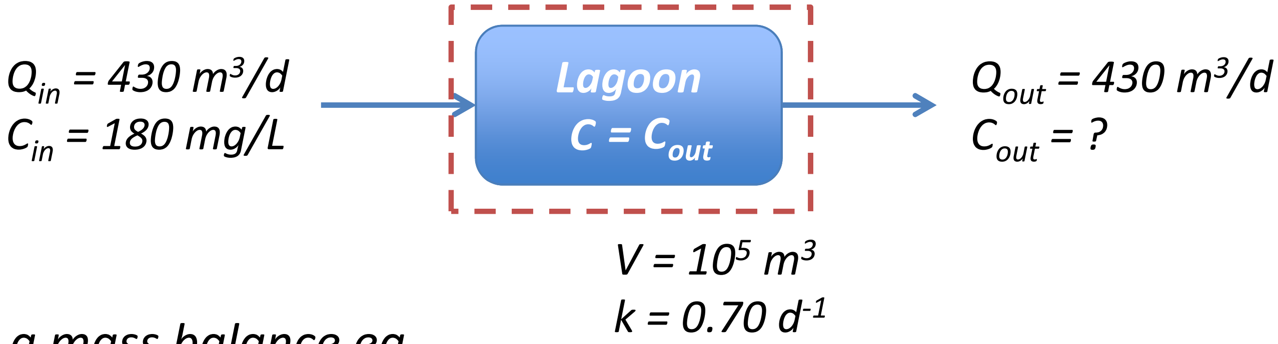
$$\Delta t = \frac{\Delta M}{d(in)/dt - d(out)/dt} = \frac{0.350\ m^3}{(1.32 - 0.32) L/min \times 10^{-3} m^3/L} = \mathbf{350\ min}$$

Water wasted = $\frac{d(out)}{dt} \times \Delta t = 0.32\ L/min \times 350\ min = \mathbf{112\ L}$

Mass balance: including reactions

Slide#10 solution)

i) Draw a schematic diagram, define CV



ii) Write a mass balance eq.

$$\cancelto{0}{\frac{dM}{dt}} = Q_{in}C_{in} - Q_{out}C_{out} - kC_{out}V$$

iii) Arrange the eq. to a useful form

$$C_{out} = \frac{Q_{in}C_{in}}{Q_{out}+kV} = \frac{430\ m^3/d \times 180\ mg/L \times 10^3\ L/m^3}{430\ m^3/d + 0.70\ d^{-1} \times 10^5\ m^3} = 1100\ mg/m^3 = \mathbf{1.1\ mg/L}$$

Reactor analysis - CMBR, 1st order reaction

Slide#14 solution)

$$-kt = ln\frac{C_{final}}{C_{initial}}$$

$$k = -\frac{1}{t}\cdot ln\frac{C_{final}}{C_{initial}} = -\frac{1}{15\ d}\cdot ln\frac{132}{280} = 0.0501\ d^{-1}$$

$$t_{99\%} = -\frac{1}{k}\cdot ln\frac{C_{final}}{C_{initial}} = -\frac{1}{0.0501\ d^{-1}}\cdot ln0.01 = \mathbf{91.9\ days}$$