Materials balances
Reactors I

Today's lecture

- Materials balances (mass balances)
- 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 balances (materials balances)

Q: In a week Prof. Choi's family purchase and bring into their house 50 kg of consumer goods. Of this amount, 50% is consumed as food. The Choi family recycle 25% of the solid waste that is generated. 1 kg accumulates in the house. Estimate the amount of solid waste they place outside their house every week.

Mass balances: 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) Solve the equation

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,

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

Mass balances: efficiency

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

mass flow rate out

mass flow rate in

- Efficiency, η

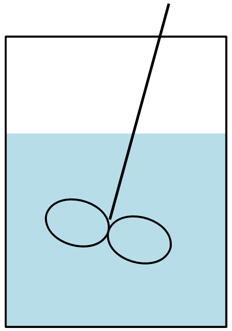
$$\eta=\frac{(mass\ in)(mass\ out)}{(mass\ in)}\times 100(\%)$$

when Q_{in} = Q_{out},

$$\eta=\frac{C_{in}-C_{out}}{C_{in}}\times 100(\%)$$

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

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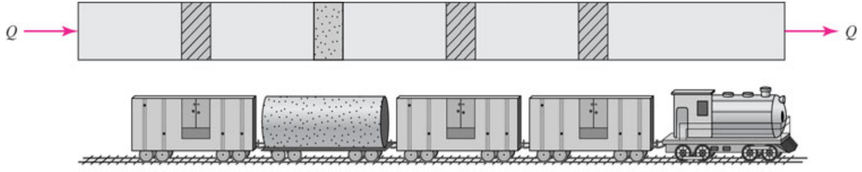


(b)

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, $r = -kC$

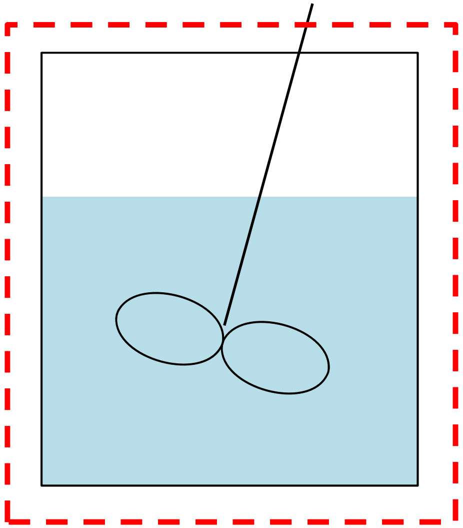
(most common in the environment)

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.

Reactor analysis – CMBR, 1st order reaction

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



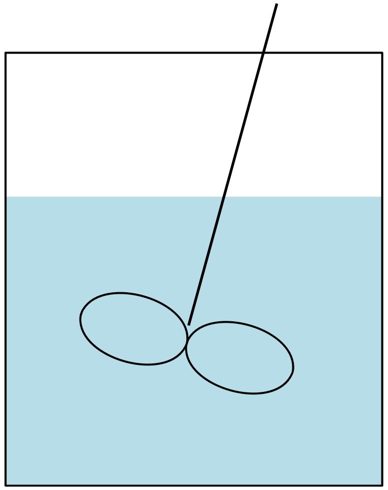
1) define control volume

2) write a mass balance eq.

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

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

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



3) solve the equation

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

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

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

Reactor analysis - CMBR, 1st 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/L)
1	280
16	132

Reading assignment

- Textbook Ch4 p. 144-162