

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:

$$(\text{Accumulation}) = (\text{Input}) - (\text{Output})$$

like in your bank account,

balance = deposit - withdrawal

Mass balance: Time as a factor

$$\left[(\text{Accumulation}) = (\text{Input}) - (\text{Output}) \right] / (\text{time})$$

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

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:

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

$C = \text{concentration [M/L}^3\text{]}$
 $Q = \text{flow rate [L}^3\text{/T]}$

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]

$$= rV \quad (V: \text{volume})$$

reaction rate, $r = -kC^n$ [M/L³/T] (n =reaction order)

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

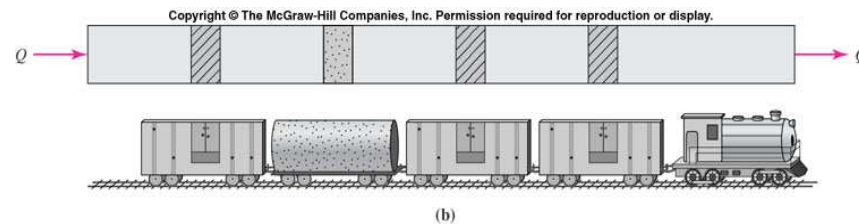
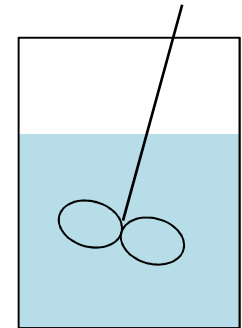
(most common in the environment)

Mass balance: including reactions

Q: A well-mixed sewage lagoon is receiving 430 m³/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 pollutant 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

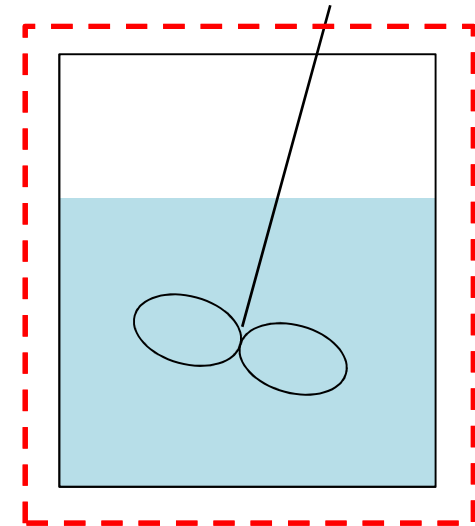


Reactor analysis – CMBR, 1st order reaction

- **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.



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

$\leftarrow -kCV$

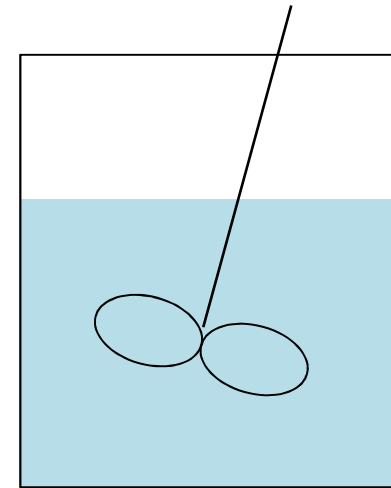
Reactor analysis - CMBR, 1st order reaction

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, 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/kg)
1	280
16	132

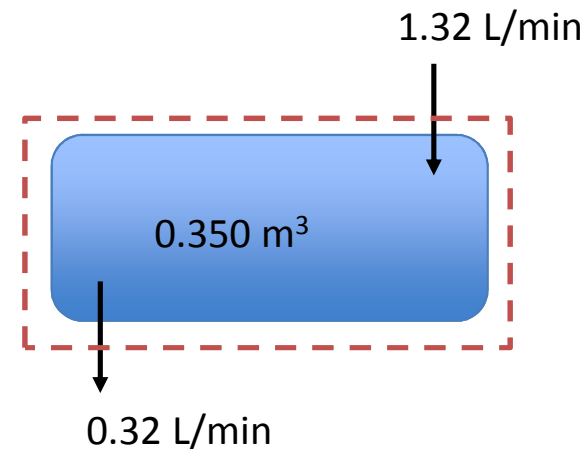
Reading assignment

- 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:

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

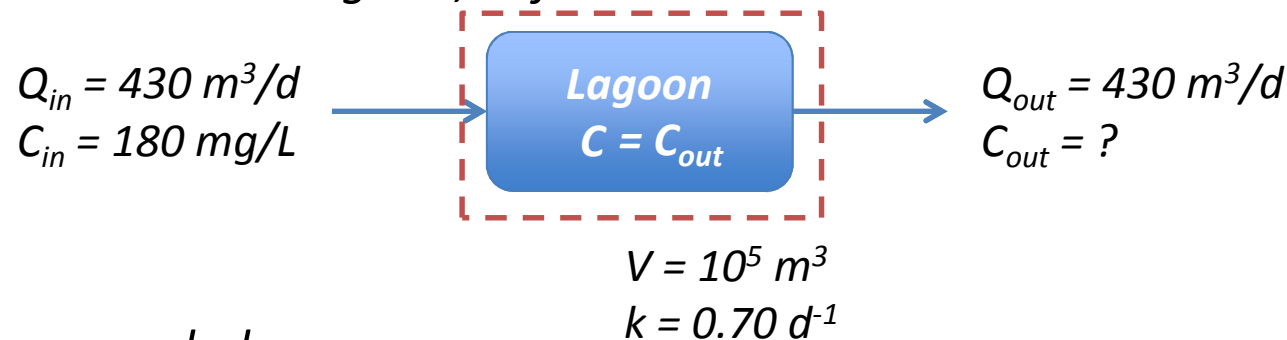
$$\Delta t = \frac{\Delta M}{d(in)/dt - d(out)/dt} = \frac{0.350 \text{ m}^3}{(1.32 - 0.32) \text{ L/min} \times 10^{-3} \text{ m}^3/\text{L}} = \mathbf{350 \text{ min}}$$

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

Mass balance: including reactions

Slide#10 solution)

i) Draw a schematic diagram, define CV



ii) Write a mass balance eq.

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

iii) Arrange the eq. to a useful form

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

Reactor analysis - CMBR, 1st order reaction

Slide#14 solution)

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

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

$$t_{99\%} = -\frac{1}{k} \cdot \ln \frac{C_{final}}{C_{initial}} = -\frac{1}{0.0501 d^{-1}} \cdot \ln 0.01 = \mathbf{91.9 days}$$