Mass and Energy Transfer

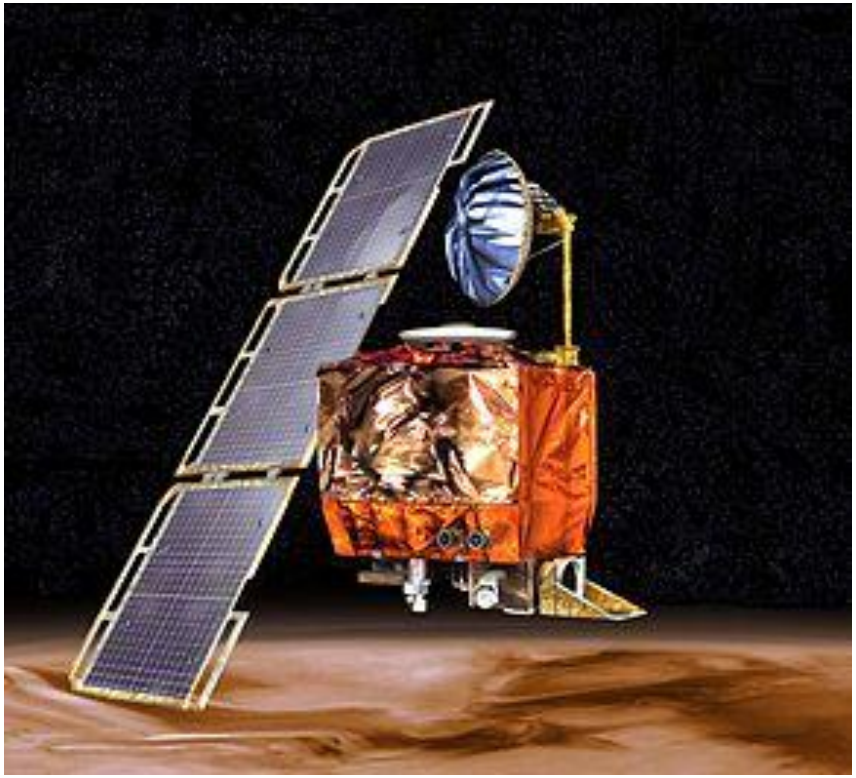
Changha Lee

School of Chemical and Biological Engineering
Seoul National University

Units of Measurement

In 1999 NASA lost a $125 million Mars orbiter because a Lockheed Martin engineering team used **English units** of measurement while the agency's team used the more **conventional metric system** for a key spacecraft operation

"The units mismatch prevented navigation information from transferring between the Mars Climate Orbiter spacecraft team at Lockheed Martin in Denver and the flight team at NASAs Jet Propulsion Laboratory in Pasadena, California" –CNN



Units of Measurement

- SI (metric) and English units

TABLE 1

Some Basic Units and Conversion Factors

Quantity	SI units	SI symbol	× Conversion factor	= USCS units
Length	meter	m	3.2808	ft
Mass	kilogram	kg	2.2046	lb
Temperature	Celsius	°C	1.8 (°C) + 32	°F
Area	square meter	m^2	10.7639	ft^2
Volume	cubic meter	m^3	35.3147	ft^3
Energy	kilojoule	kJ	0.9478	Btu
Power	watt	W	3.4121	Btu/hr
Velocity	meter/sec	m/s	2.2369	mi/hr
Flow rate	$meter^3/sec$	m^3/s	35.3147	ft^3/s
Density	$kilogram/meter^3$	kg/m^3	0.06243	lb/ft^3

Units of Measurement

TABLE 2

Common Prefixes

Quantity	Prefix	Symbol
10^{-15}	femto	f
10^{-12}	pico	p
10^{-9}	nano	n
10^{-6}	micro	μ
10^{-3}	milli	m
10^{-2}	centi	c
10^{-1}	deci	d
10	deka	da
10^{2}	hecto	h
10^{3}	kilo	k
10^{6}	mega	M
10^{9}	giga	G
10^{12}	tera	T
10^{15}	peta	P
10^{18}	exa	E
10^{21}	zetta	Z
10^{24}	yotta	Y

Concentration

✓ **Concentration:**

Amount of a specified substance in a unit amount of another substance

May be generally expressed as:

- mass/mass (pollutant in soil)
- volume/volume (pollutant in air)
- volume/mass (dose of medicine)
- mass/volume (pollutant in water)

Also refer to

- 1 ppm = 1 part in 10^6 parts
- 1 ppb = 1 part in 10^9 parts
- 1 ppt = 1 part in 10^{12} parts

- 1 % = 1 part in 100 parts

  e.g., %, wt%, % v/v, %w/w, % w/v

Concentration in Liquids

- Generally given as mass per volume.
  - mg/L
  - µg/L

- May also be expressed as weight ratio.

  Since density of water ≈ 1 g/mL ≈ 1 kg/L

$$
\begin{aligned}
1\ \text{mg/L} &= 1\ \text{mg substance} / 1\ \text{liter of water} \\
&= 1\ \text{mg substance} / 1\ \text{kg water} \\
&= 1\ \text{g substance} / 10^6\ \text{g water} \\
&= \underline{1\ \text{ppm}}
\end{aligned}
$$

- For chemicals

  Molar concentration: mole/L = M

  Mole = Weight/MW

Examples

- 23 µg of sodium bicarbonate ($NaHCO_3$) is added to 3 liters of water. What is the concentration in µg/L and in ppb (parts per billion)?

- 94 µg of phenol is added to 2 liters of water. What is the concentration in mM?

Concentration in Air

- Customarily, *volume* ratios are used for gaseous pollutants (this minimizes temperature effects).

  ppm for air is different than ppm for water:

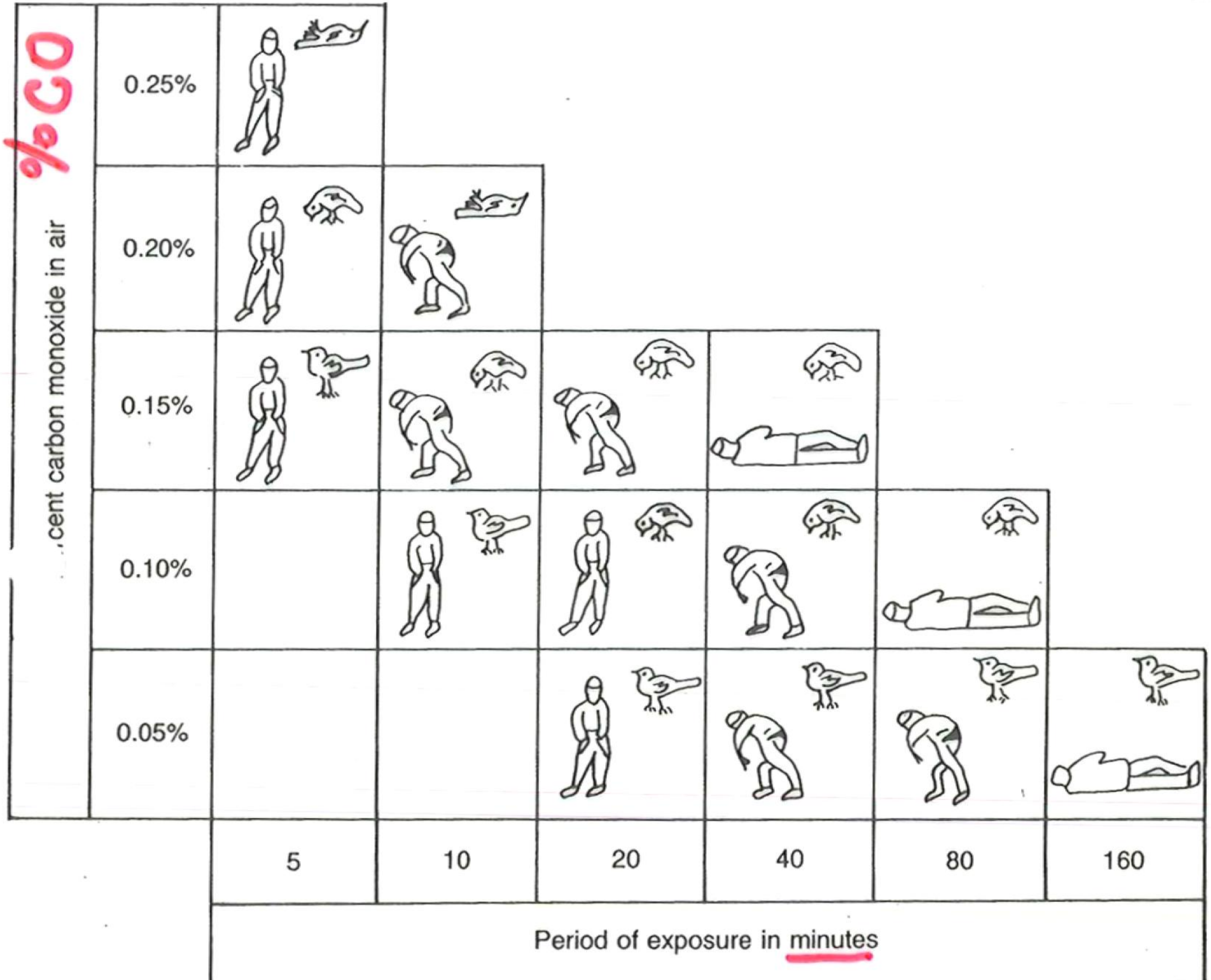
  water - ppm (by weight)

  air - ppm (by volume, ppm_v)
- But, sometimes weight/volume concentration units are used (e.g., mg/m^3)

- e.g.,

  A car is running in a closed garage. Over 30 minutes, it expels 3 ft^3 of CO.

  The garage is 20 ft by 15 ft by 15 ft. What is the resulting concentration of CO?



% CO
.cent carbon monoxide in air
0.25%
0.20%
0.15%
0.10%
0.05%
5
10
20
40
80
160
Period of exposure in minutes

Ideal Gas Law

- If gas molecules do not react with each other,
  T and P are directly proportional to each other, V is inversely proportional to T.

  PV=nRT

  - P = pressure (atm, psi, Pa, bar, in. Hg, etc)
  - V = volume (m^3, L, etc.)
  - n = number of moles
  - R = gas constant = 0.08205 atm-L-mol^{-1}-K^{-1}
  - T = absolute temperature (degrees Kelvin, K)

- At 0 °C (273 K) & 1 atm.
  - **Standard temperature and pressure, STP**
  - 1 mole occupies <u>22.4 L</u>
- At 25 °C (298 K) & 1 atm.
  - Room temperature
  - 1 mole occupies 24.5 L

Example

- A car is running in a closed garage. Over 30 minutes, it expels 3 moles of CO.

  The garage is 20 ft by 15 ft by 15 ft.

  What volume will be occupied by CO?

  What will be the concentration in ppm?

  *Assume 25℃ (room temperature) and P = 1 atm.

Approx. 1 m = 3.2 ft, 1 L = 0.035 ft^3

Mass Balance

✓ **Expression of the law of mass balance (material balance)**

- Important to assess fate and transport of pollutants and design treatment reactors

- Many approaches to solving these problems
  – Translating problem statement into correct diagram is key

- Many different types of systems
  – Steady State and Conservative Pollutant
  – Steady State and Non-Conservative Pollutant
  – Transient System

Basic Concept

✓ **Input = output + decay + accumulation**

- Steady-state implies **accumulation = 0**

- Time invariant, the concentration remains constant with time at a given point in the system, typically requiring constant inputs and outputs, although it can vary spatially from one point to another.

Steady state ≠ equilibrium

- Conservative implies **decay = 0**

- The pollutant may be recalcitrant to biological or chemical degradation, or it may be in chemical equilibrium.

Steady State and Conservative Pollutant

- This is the simplest system

$$\text{Input} = \text{output} + \underbrace{\cancel{\text{decay}}}_{0} + \underbrace{\cancel{\text{accumulation}}}_{0}$$

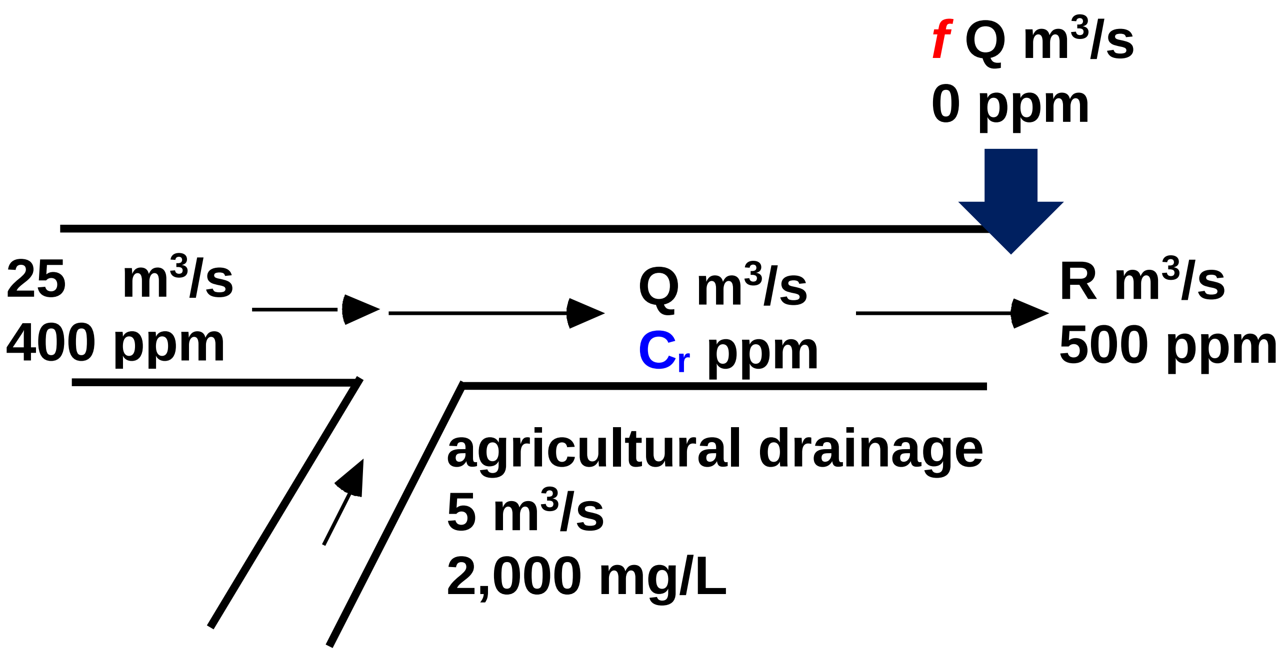
  – The pollutant does not react (conservative).
  – Concentration does not vary with time (steady-state).

- Basic equation of material balance:
  – Usually given as rates, but could also mean mass.
  Mass flow rate = $\underset{(L^3/T)}{Q} \times \underset{(M/L^3)}{C}$

- Write equation ***input = output*** for overall system and components, then solve.

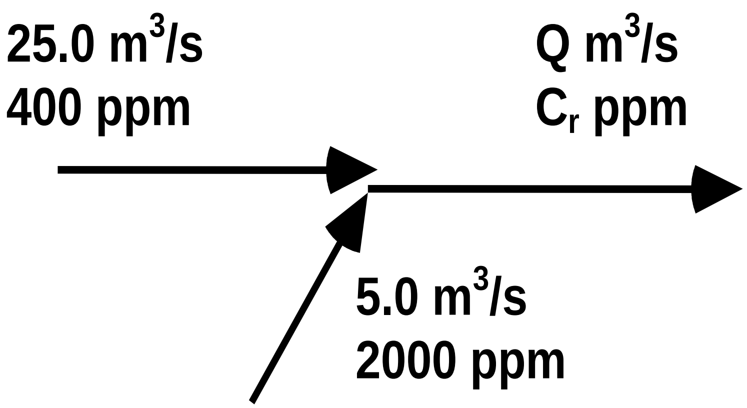
Example

- River with salt serves as water supply.
  For drinking, salt ≤ 500 ppm.
  To this end, supply is diluted with fresh water.
  How much fresh water is needed to dilute Q?



Example (solution)

To simplify break this into two domains: drainage confluence and intake points
Write equations for water flows and for salt at confluence:



$$In = Out$$

$$Overall\ flows:$$

$$25\ m^3/s + 5\ m^3/s = Q\ m^3/s$$

$$Q = 30\ m^3/s$$

$$Salt\ balance:$$

$$(25\ m^3/s)(400\ ppm) + (5\ m^3/s)(2000\ ppm)$$

$$= (Q\ m^3/s)(Cr\ \text{ppm})$$

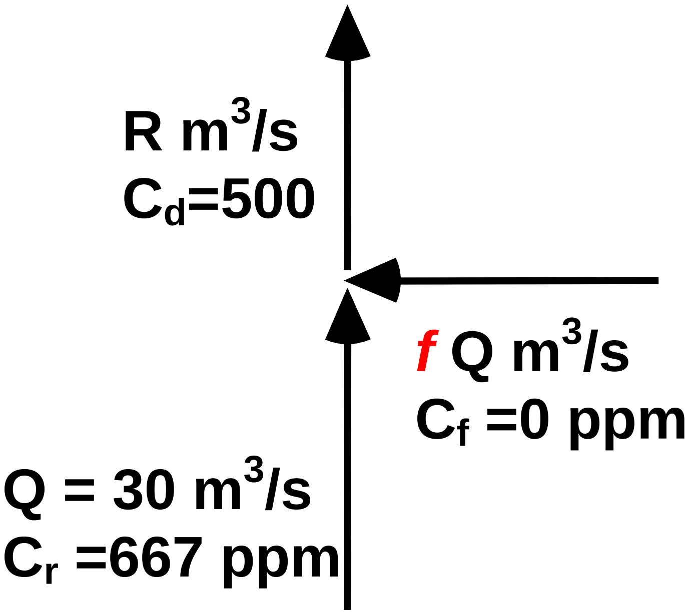
$$Q = 30\ m^3/s;$$

$$C_r = \frac{(25)(400) + (5)(2000)}{30}$$

$$C_r = 667\ \text{ppm}$$

Example (solution)

Solve the other part of the system (intake)



$In = Out$

$Material\ \ Balance:$

Steady State and Non-conservative Pollutant

√ **What if a pollutant decays by chemical and biological processes?**

- **Input = Output + <u>Decay</u>**

- Assume decay rate is proportional to concentration (1st order decay)

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

k = reaction rate constant (units = time^{-1})

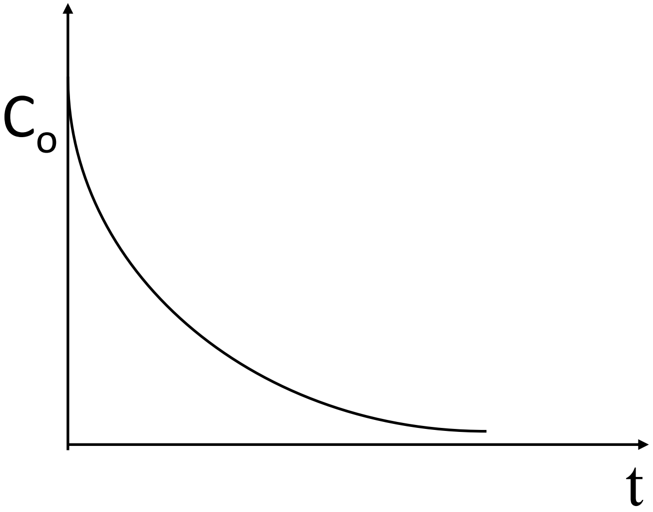
The order of the reaction refers to the exponent to which the independent variable is raised

Steady State and Non-conservative Pollutant

- Integrate: $$\frac{dC}{C} = -kdt \Rightarrow \int_{C_o}^{C} \frac{dC}{C} = -\int_0^t kdt$$

- For a **batch** system, the solution is:

$$C = C_0 e^{-kt}$$



- We will see this exponential form again, and often.

Steady State and Non-conservative Pollutant

- We are interested in the decay rate (mass/time)

  $$-dM/dt = -d(CV)/dt = V(-dC/dt) = V(kC)$$

  k has units of time^{-1}

  C has units of mass/volume

  V has units of volume

- Decay rate = *k*CV (mass/time), assumes completely mixed, incompressible fluid.

- Material balance equation:

  Input rate = Output rate + *k*CV

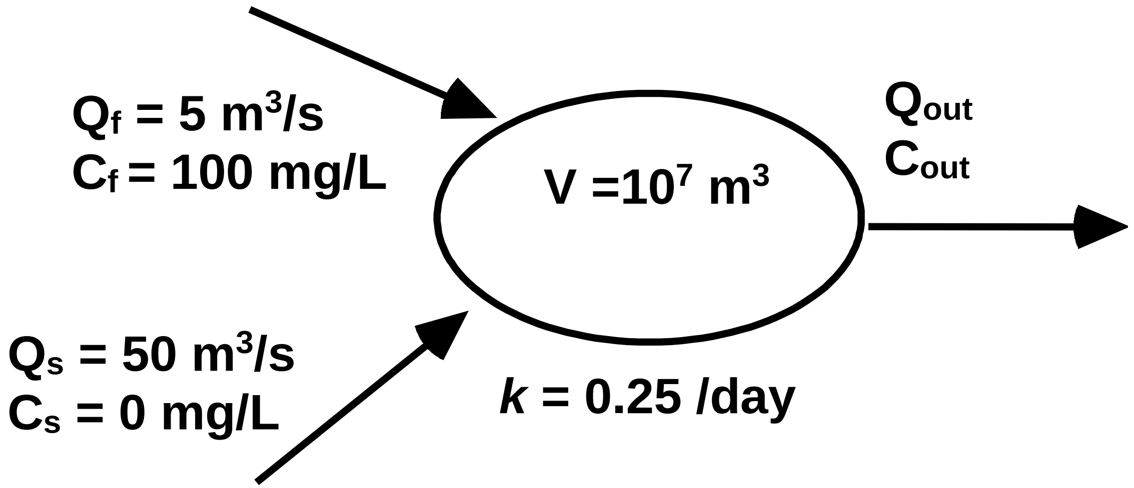
Example

- A lake with a constant volume of 10^7 m^3 is fed by a clean stream at a flow of 50 m^3/s. A factory dumps 5 m^3/s of a non-conservative waste at 100 mg/L into the lake. The pollutant has a decay rate coefficient (*k*) of 0.25 /day.

Find the steady state concentration of the pollutant in the lake.

Example (solution)

Start by drawing a diagram.



The lake has a constant volume.

Thus, for water balance:

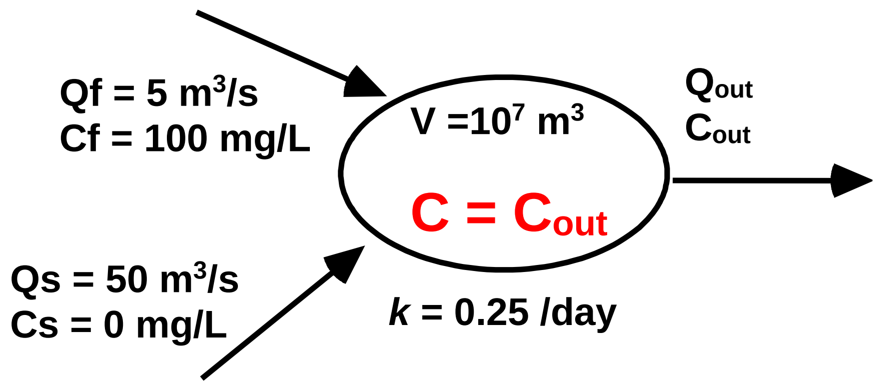
Outflow = Inflow

Example (solution)

$$In = Out$$

$$Flow\ Balance: Q_{in} = Q_{out}$$

$$Material\ \ Balance:$$



Assuming the lake is completely mixed,
C (in the lake) = C_{out}

Note: *k* was converted from d^{-1} to s^{-1}.

Transient System

√ **Consider the followings:**

- A lake with initially 0 concentration of the pollutant,

- A pollutant is introduced (source rate = S, mass/time).

- How is the concentration changing with time?

  A transient phenomenon - not steady state

Accumulation = Input – Output – Decay

$$\frac{VdC}{dt} = S - QC - kCV$$

- Eventually system reaches a steady state concentration, C_∞ when accumulation (dC/dt) = 0

$$0 = S - QC - kCV \quad \Rightarrow \quad C_\infty = \frac{S}{Q + kV}$$

Transient System

- Concentration as a function of time (before steady state is reached) is given by the solution to:

$$\frac{dC}{dt} = \frac{S}{V} - \frac{QC}{V} - kC$$

$$\Rightarrow \quad \frac{dC}{dt} = \frac{S}{V} - \left(\frac{Q+kV}{V}\right)C$$

$$\frac{dC}{dt} = \frac{Q+kV}{V}\left(\frac{S}{Q+kV}\right) - \left(\frac{Q+kV}{V}\right)C$$

$$\frac{dC}{dt} = \left(C - \frac{S}{Q+kV}\right)\left(\frac{-(Q+kV)}{V}\right)$$

but $\frac{S}{Q+kV} = C_{\infty}$ from the previous slide

$$\frac{dC}{dt} = (C - C_{\infty})\left(\frac{-(Q+kV)}{V}\right)$$

Transient System

- To integrate, we change variables:

Let y = C – C$_\infty$ $\Rightarrow$ $$\frac{dy}{dt} = \frac{dC}{dt} = (C - C_\infty)\left(\frac{-(Q + kV)}{V}\right)$$

$$\text{Thus, } \frac{dy}{dt} = -\left[k + \frac{Q}{V}\right]y$$

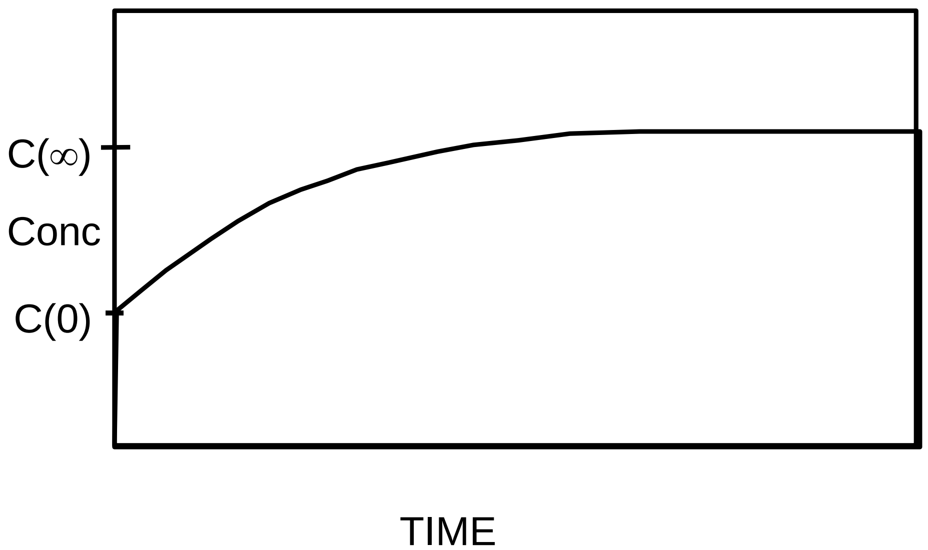
$$\Rightarrow y = y_0 e^{-\left[k + \frac{Q}{V}\right]t}$$

$$\boxed{C(t) = [C(0) - C(\infty)]e^{-(k + Q/V)t} + C(\infty)}$$

Valid for transient, completely mixed systems with pollutants following the first-order (exponential) decay

Transient System

- General Shape of this equation:



- At time = 0
  - Exponential term goes to 1
  - $C = C_0$

$$C(t) = [C(0) - C(\infty)]e^{-(k+Q/V)t} + C(\infty)$$

1

- At time = ∞
  - Exponential term goes to 0
  - $C = C_\infty$

$$C(t) = [C(0) - C(\infty)]e^{-(k+Q/V)t} + C(\infty)$$

0

Example

- A bar with a volume of 500 m^3
  Fresh air enters at a rate of 1000 m^3/hr.
  The bar is clean when it opens at 5 pm.
  Formaldehyde (HCHO) is emitted at 140 mg/hr after 5pm
  k = 0.40 /hr

  What is the concentration of HCHO at 6 pm? (t = 1h)

Example (solution)

- Governing equation:

$$C(t) = [C(0) - C(\infty)]e^{-(k+Q/V)t} + C(\infty)$$

Given:

- Q =
- V =
- S =
- k =
- C_0 =

Example (solution)

- Find C_∞, the steady state concentration of HCHO

$$C_\infty = \frac{S}{Q + kV}$$

$$=$$

$$=$$

This represents the maximum concentration that would be reached

- Interested in the concentration at 6 PM (one hour after bar opens)

  t = 1 hr

$$C(t) = [C(0) - C(\infty)]e^{-(k+Q/V)t} + C(\infty)$$

$$C(t) = (0 - 0.117)e^{-(0.40+1000.0/500.0)t} + 0.117$$

Example (solution)

✓ What if ***k* = 0**?

- Need to recalculate C_∞

$$C(\infty) = \frac{S}{Q + kV}$$

- After 1 hr,

$$C(t) = [C(0) - C(\infty)]e^{-(k + Q/V)t} + C(\infty)$$

Example (solution)

✓ What if **Q = 0**?

- Recalculate C_∞

$$C(\infty) = \frac{S}{Q + kV}$$

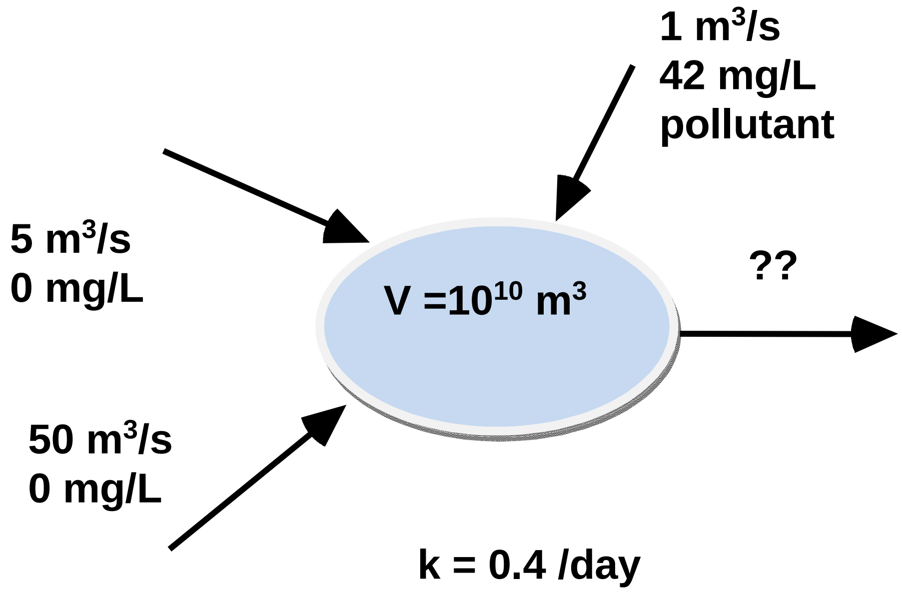
- After 1 hr,

$$C(t) = [C(0) - C(\infty)]e^{-(k + Q/V)t} + C(\infty)$$

Example

- A new factory opens discharging a pollutant at $1 m^3/s$, 42 mg/L to the lake in the following flow scheme.

If *k* is 0.4/day, what is the concentration after 1 week?



Example (solution)

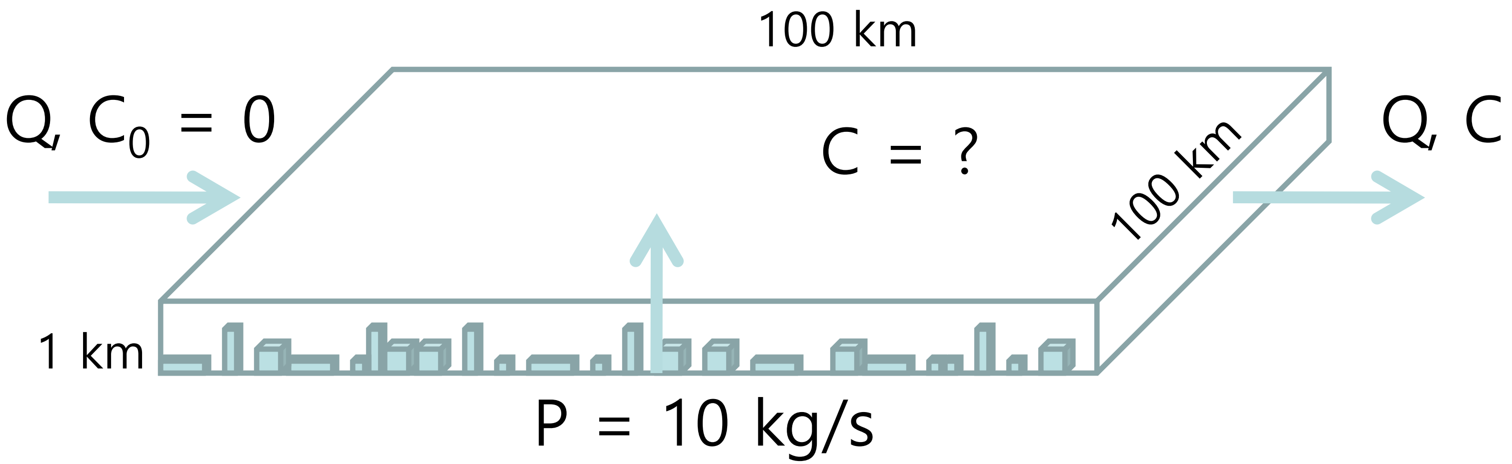
- First, determine C_∞

$$C_\infty = \frac{S}{Q + kV}$$

- After 7 days, $C(t) = [C(0) - C(\infty)]e^{-(k + Q/V)t} + C(\infty)$

Example – Urban Air Pollution (Box Model)

- What is the steady-state concentration of the pollutant?



- k = 0.2 h^{-1} = 5.56 x 10^{-5} s^{-1}
- Horizontal wind speed: u = 4 m/s

Example (solution)

- Note:

  Q has units of volume / time = length^3 / time

  u has units of length / time

  A has units of length^2

  Therefore, Q = u*A = wind speed * cross-sectional area

  Q = (4 m/s)(100 x 1 km^2) x 1 km / 1000 m = 0.4 km^3/s

- Mass balance

$$0 = [QC_0 + P] - QC - kCV$$

$$0 = [0 + 10\frac{kg}{s}] - (0.4\ \frac{km^3}{s}) * C - (5.56 \times 10^{-5} s^{-1}) * C * (100 \times 100 \times 1\ km^3)$$

$$0 = 10\frac{kg}{s} - 0.4\frac{km^3}{s}C - 0.556\frac{km^3}{s}C$$

$$0 = 10\frac{kg}{s} - 0.96\frac{km^3}{s}C$$

$$\Rightarrow C = \frac{10}{0.96} = 10.4\frac{kg}{km^3}$$

$$\underline{= 10.4\frac{\mu g}{m^3}}$$

Example

- Corn is used to make alcohol.

Input is 800 kg/h of corn into still, it contains 11.3% alcohol, 83.9% water, and inert materials. Finished product is 12.6% of feed (by mass) and contains 73.1% alcohol, 26.2% water, and 0.7% inert.

What is quantity and composition of the bottoms?

Example (solution)

First, diagram:

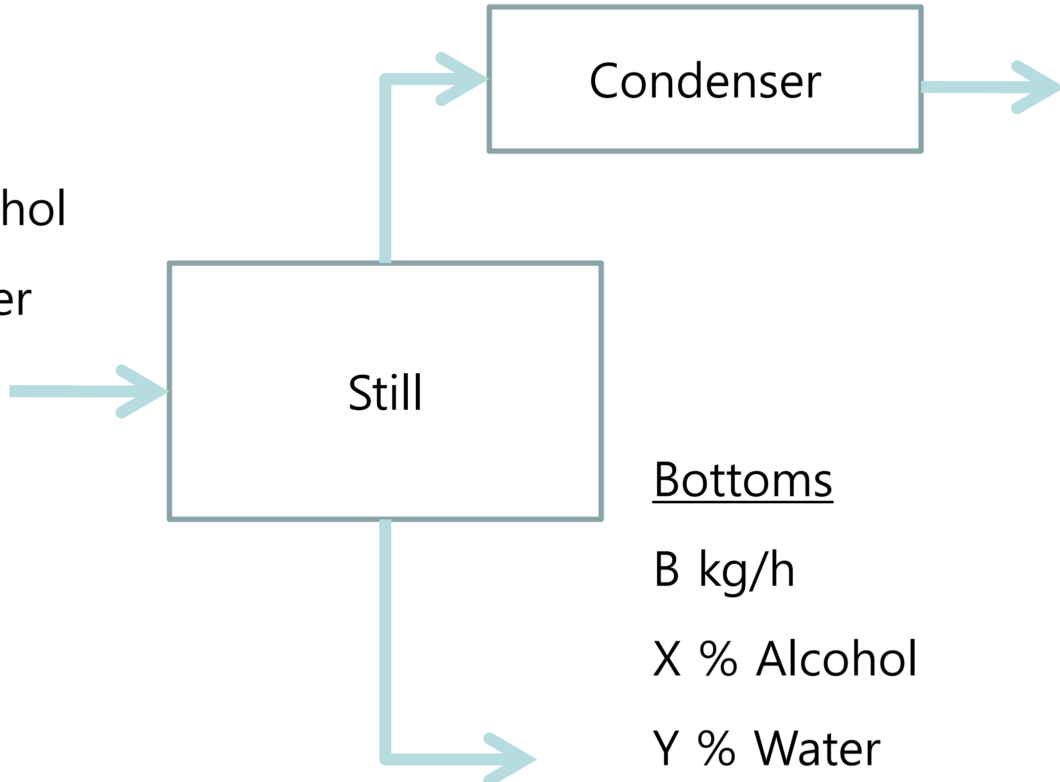
<u>Corn Feed</u>

800 kg/h

11.3 % Alcohol

83.9 % Water

4.8 % Inert



<u>Product</u>

(0.126)(800) =

100.8 kg/h

73.17 % Alcohol

26.20 % Water

0.7 % Inert

<u>Bottoms</u>

B kg/h

X % Alcohol

Y % Water

Z % Inert

Example (solution)

- Input = Output

- Overall Balance:

$$\boxed{\begin{aligned} &800 = 100.8 + B \\ &\underline{B = 699.2\ kg / h} \end{aligned}}$$

- Alcohol Balance:

$$\boxed{\begin{aligned} &(0.113)(800) = (0.731)(100.8) + \frac{X}{100}(699.2) \\ &90.4 = 73.685 + (X)(6.992) \\ &\underline{X = 2.39\ \%} \end{aligned}}$$

Example (continued)

- Water Balance:

$$(0.839)(800) = (0.262)(100.8) + \frac{Y}{100}(699.2)$$

$$\underline{Y = 92.22\ \%}$$

- Then, inert

$$Z = 100 - X - Y$$

$$Z = 100 - 2.39 - 92.22$$

$$\underline{Z = 5.39\ \%}$$

- Therefore, Bottoms:
  - 699.2 kg/h
  - 2.39 % Alcohol
  - 92.22 % Water
  - 5.39 % Inert