Lecture 3
Mass Balances in *Continuously Stirred Tank Reactor* (CSTR)

- To use 'mass balances' to develop steady and non-steady analytical solutions for CSTR-like systems (e.g., natural lakes and impoundments)
- Steady-state solutions to MBDE:
  - a) transfer function and
  - b) residence time
- Non-steady state solutions to MBDE:
  - a) Eigenvalues,
  - b) general solutions, and
  - c) particular solution

Mass balance of a Well-Mixed Lake

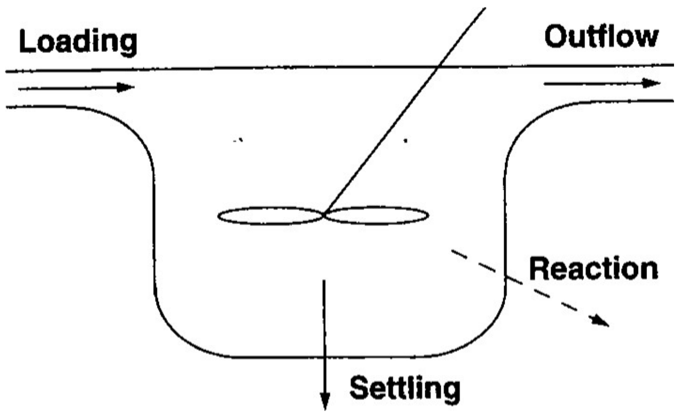
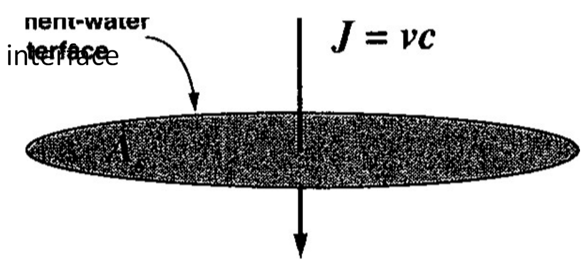


FIGURE 3.1

A mass balance for a well-mixed lake. The arrows represent the major sources and sinks of the pollutant. The dashed arrow for the reaction sink is meant to distinguish it from the other sources and sinks, which are transport mechanisms.



Sediment-water

FIGURE 3.2

Settling losses formulated as a flux of mass across the sediment-water interface.

Mass Balance for a Well-mixed Lake (CSTR-like)

Example of balance of rates for a well-mixed lake:

Accumulation rate =

loading rate – outflow rate – reaction rate – settling rate

or

$$V(dc/dt) = W(t) - Qc - kVc - \nu A_s c$$

where

W(t) represents all loadings to the lake (i.e., total Q and average Cin) and the settling rate is modeled by $\nu A_s c$ (= $k_s Vc$ with $k_s = \nu/H$)

(Cont.)

- Accuml'n rate: change of mass, m, in the defined system or part of it over time t.
- Loading rate: mass enters a system from sources.
- Outflow rate: mass carried from the system by outflow streams.
- Reaction rate: mass of pollutant produced or consumed in water
- Settling rate: flux of mass lost across the sediment-water interface.

(Cont.)

- loading $= W(t) = Qc_{in}$
- reaction $= kM = kVc$
- settling $= \nu A_s c = k_s V c$
- outflow $= Qc$

(Cont.)

- Model predicts concentration as a function of time.
- Time is an independent variable.
- Concentration is a dependent variable.
- W(t) is the forcing function since it ‘forces’ the system.
- V, Q, k, ν and A_s are parameters (or coefficients).

Steady State Solutions

If the accumulation rate is 0 or "nil": $dc/dt = 0$

$$c = W/(Q+kV+\nu A_s)$$

where

$$c = (1/a)\ W$$

$$a = (Q+kV+\nu A_s)$$

Thus, concentration is a function of loading, and depends on the physics, chemistry and biology of the aquatic system!!!

Example 3.1: Steady-State Solution – CSTR (i.e., Lake)

EXAMPLE 3.1. MASS BALANCE. A lake has the following characteristics:

Volume = 50,000 m^3
Mean depth = 2 m
Inflow = outflow = 7500 $m^3\ d^{-1}$
Temperature = 25°C

The lake receives the input of a pollutant from three sources: a factory discharge of 50 kg d^{-1}, a flux from the atmosphere of 0.6 g $m^{-2}\ d^{-1}$, and the inflow stream that has a concentration of 10 mg L^{-1}. If the pollutant decays at the rate of 0.25 d^{-1} at 20°C (θ = 1.05),

(*a*) Compute the assimilation factor.
(*b*) Determine the steady-state concentration.
(*c*) Calculate the mass per time for each term in the mass balance and display your results on a plot.

Solution: (*a*) The decay rate must first be corrected for temperature (Eq. 2.44):

$$k = 0.25 \times 1.05^{25-20} = 0.319\,d^{-1}$$

Then the assimilation factor can be calculated as

$$a = Q + kV = 7500 + 0.319(50{,}000) = 23{,}454\ m^3\ d^{-1}$$

Notice how the units look like flow (that is, volume per time). This is because the same mass units are used in the numerator and the denominator and they cancel, as in

$$\frac{g\ d^{-1}}{g\ m^{-3}} \rightarrow m^3\ d^{-1}$$

EXAMPLE 3.1. MASS BALANCE. A lake has the following characteristics:

Volume $= 50{,}000\ \text{m}^3$
Mean depth $= 2\ \text{m}$
Inflow $=$ outflow $= 7500\ \text{m}^3\ \text{d}^{-1}$
Temperature $= 25°\text{C}$

The lake receives the input of a pollutant from three sources: a factory discharge of $50\ \text{kg d}^{-1}$, a flux from the atmosphere of $0.6\ \text{g m}^{-2}\ \text{d}^{-1}$, and the inflow stream that has a concentration of $10\ \text{mg L}^{-1}$. If the pollutant decays at the rate of $0.25\ \text{d}^{-1}$ at 20°C ($\theta = 1.05$),

(*a*) Compute the assimilation factor.
(*b*) Determine the steady-state concentration.
(*c*) Calculate the mass per time for each term in the mass balance and display your results on a plot.

Solution: (*a*) The decay rate must first be corrected for temperature (Eq. 2.44):

$$k = 0.25 \times 1.05^{25-20} = 0.319\ \text{d}^{-1}$$

Then the assimilation factor can be calculated as

$$a = Q + kV = 7500 + 0.319(50{,}000) = 23{,}454\ \text{m}^3\ \text{d}^{-1}$$

Notice how the units look like flow (that is, volume per time). This is because the same mass units are used in the numerator and the denominator and they cancel, as in

$$\frac{\text{g d}^{-1}}{\text{g m}^{-3}} \rightarrow \text{m}^3\ \text{d}^{-1}$$

(*b*) The surface area of the lake is needed to calculate the atmospheric loading

$$A_s = \frac{V}{H} = \frac{50{,}000}{2} = 25{,}000 \text{ m}^2$$

The atmospheric load is then computed as

$$W_{\text{atmosphere}} = JA_s = 0.6(25{,}000) = 15{,}000 \text{ g d}^{-1}$$

The load from the inflow stream can be calculated as

$$W_{\text{inflow}} = 7500(10) = 75{,}000 \text{ g d}^{-1}$$

Therefore the total loading is

$$W = W_{\text{factory}} + W_{\text{atmosphere}} + W_{\text{inflow}} = 50{,}000 + 15{,}000 + 75{,}000 = 140{,}000 \text{ g d}^{-1}$$

and the concentration can be determined as (Eq. 3.18)

$$c = \frac{1}{a}W = \frac{1}{23{,}454}140{,}000 = 5.97 \text{ mg L}^{-1}$$

(*c*) The loss due to flushing through the outlet can be computed as

$$Qc = 7500(5.97) = 44{,}769 \text{ g d}^{-1}$$

and the loss due to reaction as

$$kVc = 0.319(50{,}000)5.97 = 95{,}231 \text{ g d}^{-1}$$

These results along with the loading can be displayed as in Fig. 3.3.

Example 3.1: Detailed Mass Balance – Sources and Sinks

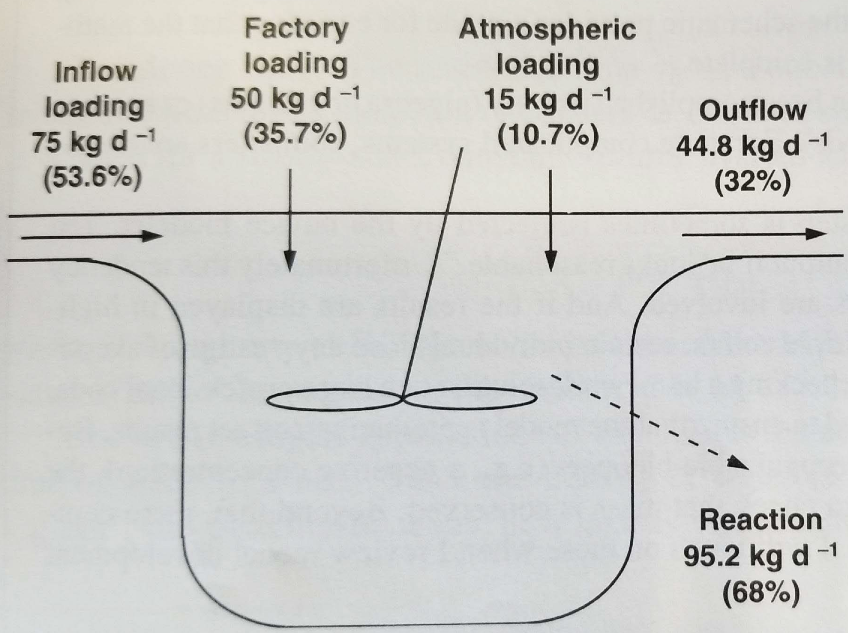


FIGURE 3.3
A mass balance for the well-mixed lake from Example 3.1. The arrows represent the major sources and sinks of the pollutant. The mass-transfer rates have also been included along with the percent of total mass inflow accounted for by each term.

Transfer Function (β):

"Indicator of the ability of a steady state system to assimilate pollutants"

If we express $W = Q\,c_{in}$, we then have that

$c/c_{in} = Q / (Q+kV+\nu A_s)$

$= \beta$ or transfer function

If $\beta \leq\leq 1$, lake has large assimilative capacity

If $\beta \rightarrow 1$, lake has low assimilative capacity

Example 3.2: Transfer Function and Residence Time

EXAMPLE 3.2. TRANSFER FUNCTION AND RESIDENCE TIMES. For the lake in Example 3.1, determine the (*a*) inflow concentration, (*b*) transfer function, (*c*) water residence time, and (*d*) pollutant residence time.

Solution: (*a*) The inflow concentration is computed as

$$c_{\text{in}} = \frac{W}{Q} = \frac{140{,}000}{7500} = 18.67 \text{ mg L}^{-1}$$

(*b*) The transfer coefficient can now be determined as

$$\beta = \frac{c}{c_{\text{in}}} = \frac{Q}{Q + kV} = 0.32$$

Thus the removal processes act to create a lake concentration that is 32% of the inflow concentration.

(*c*) The residence time can be calculated as

$$\tau_w = \frac{V}{Q} = \frac{50{,}000}{7500} = 6.67 \text{ d}$$

(*d*) The pollutant residence time is

$$\tau_c = \frac{V}{Q + kV} = \frac{50{,}000}{7500 + 0.319(50{,}000)} = 2.13 \text{ d}$$

Because of the addition of the decay term, the residence time of a pollutant is about one-third the water residence time.

Residence Time

"Amount of time required for outflow to replace water (or pollutant) in the system (lake)"

Water residence time (or "hydraulic")

$$t_w \text{ (or } t \text{ or } \tau \text{)} = V/Q$$

Pollutant residence time

$$t_c = V/(Q+kV+\nu A_s)$$

Example 3.4: Residence Time

EXAMPLE 3.4. RESPONSE TIME. Determine the 75%, 90%, 95%, and 99% response times for the lake in Example 3.3.

Solution: The 75% response time can be computed as

$$t_{75} = \frac{1.39}{0.469} = 2.96\,\text{d}$$

In a similar fashion we can compute $t_{90} = 3.9$ d, $t_{95} = 6.4$ d, and $t_{99} = 9.8$ d.

Non-steady State Solutions (temporal or dynamic behavior)

- From a mass balance, we derive that
  - $V(dc/dt) = W(t) - Qc - kVc - \nu A_s c$, which can be modified to yield
  - $dc/dt + \lambda c = W(t)/V$,
    where $\lambda = (Q/V) + k + \nu/H$ or *eigenvalue*
  - A solution for $c = c_g + c_p$,
    where c_g is the solution for $W(t) = 0$ and c_p is a solution when $W(t) \neq 0$

The General Solution and Response Time

- A general solution (C = Co at t = 0 and W(t) = 0) is
  - $C = C_o e^{-\lambda t}$
- Because λ is not a "clear value" to non-scientists and engineers, the use of a response time is used for laymen:
  - Half-life or $t_{50} = 0.693/\lambda$
  - Any $t_{\phi} = (1/\lambda) \ln [100/(100 - \phi)]$

Exponential Function & Temporal Response in CMR Lake

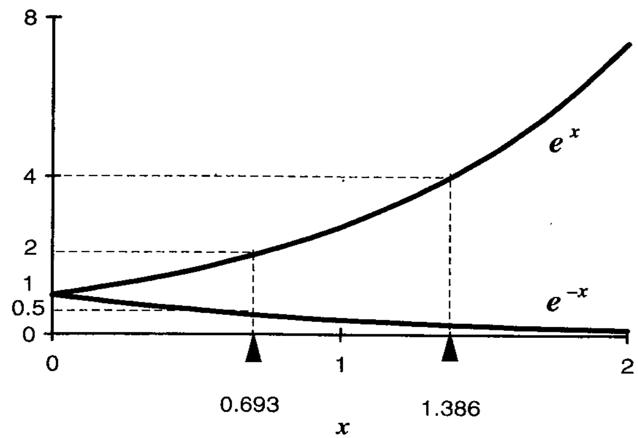


FIGURE 3.5
The exponential function.

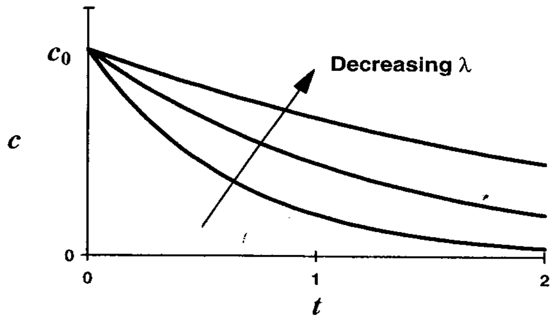


FIGURE 3.6
The temporal response of our well-mixed lake model following the termination of all loadings at $t = 0$.

Example 3.3: General Solution

EXAMPLE 3.3. GENERAL SOLUTION. In Example 3.1 we determined the steady-state concentration for a lake having the following characteristics:

Volume = 50,000 m^3
Mean depth = 2 m
Inflow = outflow = 7500 $m^3\ d^{-1}$
Temperature = 25°C
Waste loading = 140,000 g d^{-1}
Decay rate = 0.319 d^{-1}

If the initial concentration is equal to the steady-state level (5.97 mg L^{-1}), determine the general solution.

Solution: The eigenvalue can be computed as

$$\lambda = \frac{Q}{V} + k = \frac{7500}{50{,}000} + 0.319 = 0.469\ d^{-1}$$

Thus the general solution is

$$c = 5.97e^{-0.469t}$$

which can be displayed graphically as

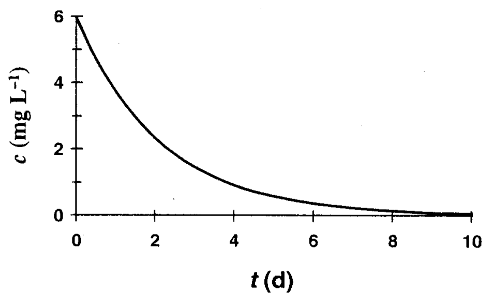


FIGURE E3.3

Note that by $t = 5$ d the concentration is reduced to less than 10% of its original value. By $t = 10$ d, for all intents and purposes, it has reached zero.