HWR 516

HYDROLOGIC TRANSPORT PROCESSES

(Yeh, 2004 Fall)

Chapter 1

Lumped Parameter Model for Surface Water Reservoirs

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Linear 1 - order Non-homogeneous O.D.E.

Consider an ordinary differential equation that has a form

$$\frac{dC}{dx} + f(x)C = r(x) \qquad (1)$$

where $r(x) \neq 0$. It has the general solution:

$$C(x) = e^{-h}\left[\int e^{h} r(x)dx + A\right] \qquad (2)$$

where $h = \int f(x)dx$

Example: Consider the following ordinary differential equation,

$$\frac{dC}{dx} - C = e^{2x} \qquad (3)$$

Compare Eq. (3) with Eq. (1), we have

$f = -1$, $r(x) = e^{2x}$, $h = \int (-1)dx = -x$

From Eq. (2), we have the general solution for the ordinary differential equation,

$$\begin{aligned} C(x) &= e^{-x}\left[\int e^{-x} e^{2x} dx + A\right] \\ &= e^{x}\left[\int e^{x} dx + A\right] \\ &= e^{x}\left[e^{x} + A\right] = e^{2x} + Ae^{x} \end{aligned} \qquad (4)$$

in which A can be determined if an initial or boundary condition is specified. Afterwards, we have a particular solution.

Concentration:

1. Volume Averaged Concentration: mass of tracer per unit volume

$$C = \frac{M}{\mathbf{V}} = \left[\frac{M}{L^3}\right] \textit{ for water, } \quad 1l = 10^6 \, mg \textit{ water}$$

$$= \underbrace{\frac{mg}{l}}_{\frac{mass}{volume}} \approx \underbrace{1ppm}_{\frac{weight}{weight\ unit}}$$

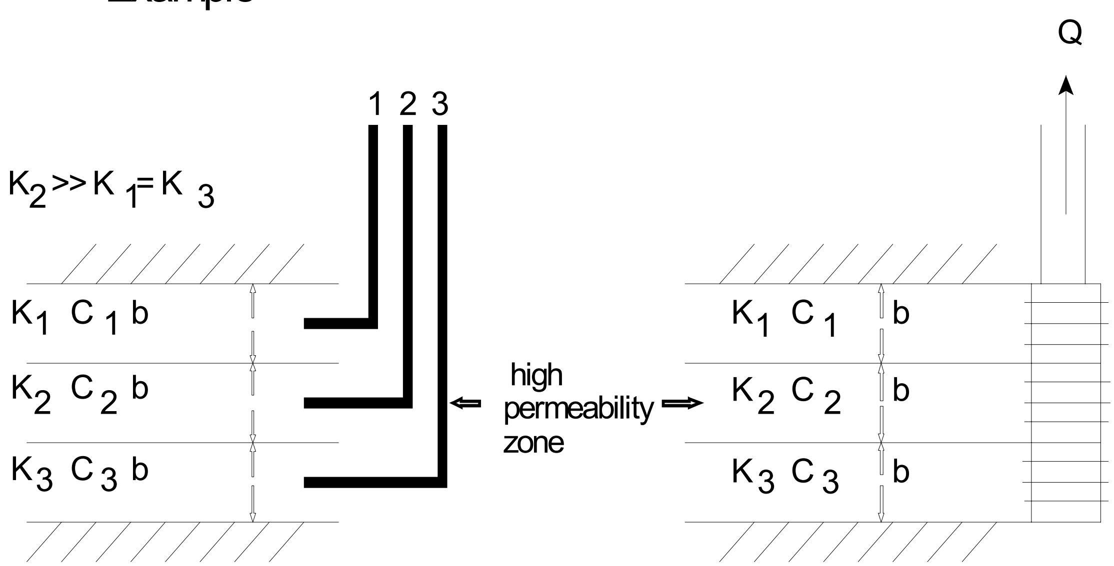
2. Flux averaged concentration:

$$C_f = \frac{\int Cu\,dA}{\int u\,dA}$$

Volume Average $\overline{C} = \frac{C_1 + C_2 + C_3}{n} = \frac{M}{\mathbf{V}}$

flux average $\overline{C}_f = \frac{Q_1C_1 + Q_2C_2 + Q_2C_2}{Q}$

Example



The highest conductive zone contributes the most to the flux averaged concentration.

See: Parker, & Van Genuchten, Flux-averaged and volume- averaged concentrations in continuum approaches to solute transport, WRR, 20, 866-872, 1984.

3. Mass-Per-Mass Units:

$$C = \frac{Mass\ of\ \alpha / Vol}{Mass\ of\ solution / Vol} = \frac{\rho_\alpha}{\rho} = \frac{Mass\ of\ \alpha}{Mass\ of\ solution}$$

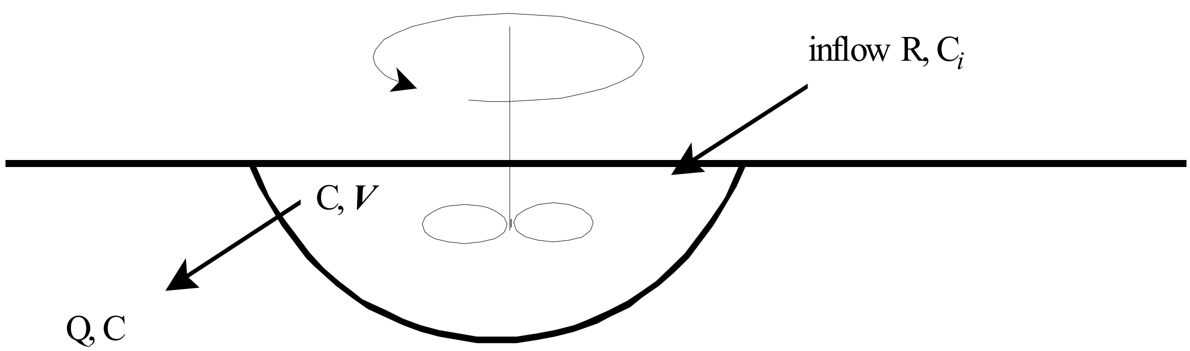
$$= ppm\,(parts\ per\ million) = 1x10^{-6}$$

Lumped Parameter Models (Well-Mixed Systems)

A lumped parameter model is a fundamental building block of any analysis of a complex system. The model aims at the balance of mass, energy, etc of a system as a function of time. It assumes that the system is well mixed and ignores any spatial variation within the system. As a result, the resultant state of the system represents only the behavior of the system on the spatial average sense. For example, applications of a lumped parameter model to study the temporal variation of water quality of bays, estuaries, or lakes assume that the extent of turbulence due to wind, tide or other forces is so great that chemicals of the system are considered to be completely mixed and uniformly distributed. Of course, this assumption likely is not true for most bays, estuaries, and lakes. In this case, the well-mixed assumption merely attempts to represent spatial averaged concentration of chemicals in these nature systems.

Lumped Parameter Model for Water Quality of Lakes:

Consider a lake as illustrated in the figure below. Inflow of any chemicals to the lake is considered well mixed with the lake water instantaneously.



where
V = total volume of the lake [L^3]
Q = outflow rate from the lake [L^3/T]
R = inflow rate to the lake [L^3/T]
Ci = inflow conc. (mass of solute) / (mass of solution, ppm)
C = outflow and lake concentration due to the well-mixed assumption
ρ = density of water

$$C = \frac{\rho_\alpha}{\rho} = \frac{mass\ of\ \alpha / vol}{mass\ of\ solution / vol} = \frac{mass\ of\ \alpha}{mass\ of\ solution} = ppm$$

Mathematical Formulation:

1. Water Balance:

change of mass = mass inflow - mass outflow

$$\frac{d\rho \boldsymbol{V}(t)}{dt} = \rho[R - Q] \tag{1}$$

If we assume that the density of water, ρ, is time invariant, the equation becomes

$$\frac{d\boldsymbol{V}}{dt} = R - Q \tag{2}$$

2. Mass Balance for an α chemical species in the lake:

$$\frac{d\rho C_\alpha \boldsymbol{V}}{dt} = \rho C_i R - \rho C Q + \rho S \boldsymbol{V} \tag{3}$$

where $\rho = \frac{M_w}{\boldsymbol{V}_w}, C_\alpha = \frac{M_\alpha}{M_w}$ and the last term in (3) represents a sink (degradation, precipitation, or other chemical reactions) or source (production) term for the chemical. Again, if ρ = constant, we then have

$$\boldsymbol{V}\frac{dC}{dt} + C\frac{d\boldsymbol{V}}{dt} = C_i R - CQ + S\boldsymbol{V} \tag{4}$$

Incorporating the water balance equation into the above equation yields

$$\boldsymbol{V}\frac{dC}{dt} + C(R - Q) = C_i R - CQ + S\boldsymbol{V} \tag{5}$$

or

$$\boldsymbol{V}\frac{dC}{dt} + CR = C_i R + S\boldsymbol{V} \tag{6}$$

Notice that V is outside the time derivative but it is a function of time, not a constant.

Now, we will consider the sink or source term in the chemical mass balance equation. For the sake of simplicity, we will assume the sink term in Eq. (6) can be described by a linear isotherm reaction model,

$$S = -kC \tag{7}$$

in which the negative sign denotes the sink (losing mass). This equation states that the amount of lost of α chemical is linearly proportional to its concentration in the lake water. The parameter k is a rate constant, [1/T].

Applications of the Lumped Parameter Model

Example (1). Consider a radioactive chemical in a closed chamber (i.e., Q = R = 0) of a volume V in which it decays. To consider the chemical mass balance, eq. (6) is simplified to

$$V\frac{dC}{dt} = SV \qquad \frac{dC}{dt} = -kC \tag{8}$$

The analytical solution to eq. (8) is

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

where C_o = initial conc. Taking logarithm of the solution yields

$$ln\frac{C}{C_o} = -kt$$

If we set C/C_0 =1/2, then we have

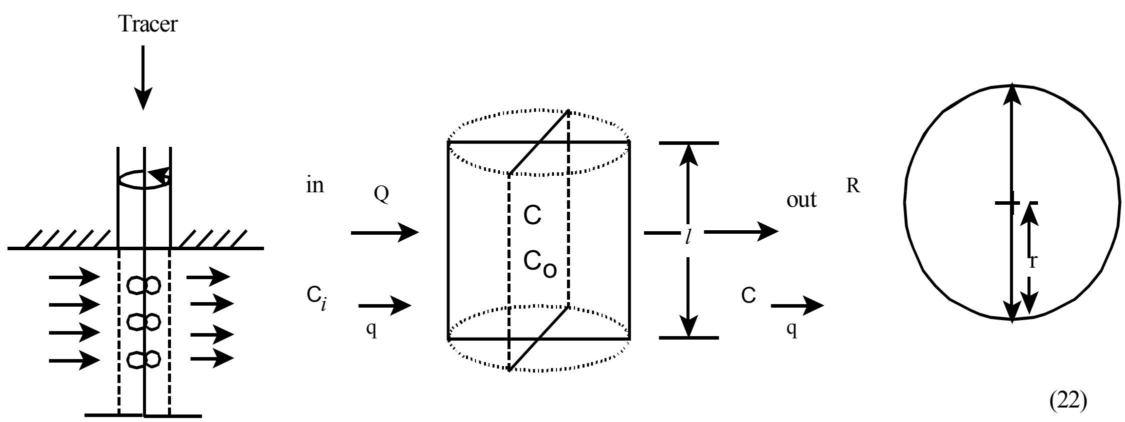
$$t_{1/2} = \frac{ln2}{k}$$

which is defined as the half-life of the chemical. In other words, it is the time required for the chemical to decay to a half of its original concentration.

Example (2): Point Dilution Method for groundwater velocity.

The lumped parameter approach has also been applied to determine groundwater velocity using a point dilution method (see Drost et al., 1968, Point dilution methods of investigating groundwater flow by means of radioisotopes, **WRR, 4,** 125-146). The point dilution method involves injection of a certain mass of a tracer into a well and monitors the change in the tracer concentration in the well. Assuming the tracer is instantaneously well mixed with the original water in the well, the concentration of the tracer in the well then decay as it is mixed with clear groundwater entering the well. Based on the rate of the decay, the rate of groundwater entering the well can be determined. If we consider the screened section of the well is the control volume (see Figure) and assume that there is no storage effect in the well, i.e.,

$$Q = R,$$



(22)

We also assume that the concentration of the tracer in the ambient groundwater is zero and the tracer is well mixed in the well at t=0.

$$C_i = 0, \quad C_o = C \qquad \text{at } t = 0$$

From Eq. (6), we have an equation that describes how the concentration in the well changes with time:

$$V\frac{dC}{dt} + CR = C_i R + SV$$

Suppose that the tracer is non-reactive. We then have

$$V\frac{dC}{dt} = -CR$$

Knowing that $\boldsymbol{V} = \pi r^2 l$ and assuming that q is uniform and the cross-sectional area, A, approximates the surface area where groundwater enter the well, we can calculate the total inflow or outflow using

$$R = q \cdot A = q \cdot 2rl$$

Thus, we have an ordinary differential equation for the average concentration of the tracer

$$\boldsymbol{V}\frac{dC}{dt} = -\frac{q \cdot 2rl}{\pi r^2 l}C = -\frac{2q}{\pi r}C$$

Let C = C_o at $t = 0$, we solve the equation for q and we have

$$q = -\frac{\pi r}{2t}\, ln\left(\frac{C}{C_o}\right)$$

The linear average velocity (magnitude) of the groundwater can then be obtained by

$$v^* = \frac{q}{n\alpha}$$

where α is a correction factor to account for our assumptions, and n is the porosity of the porous medium. A similar equation can also be formulated for any heat pulses for determining groundwater velocity in a well.

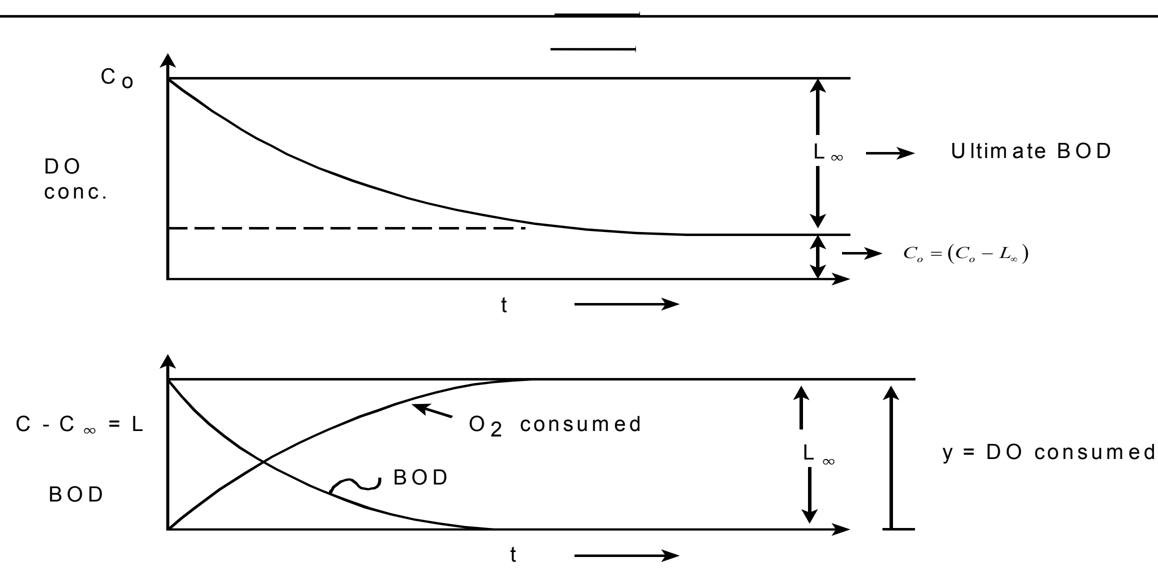
Example (3): BOD (Biochemical Oxygen Demand)

See Thomann & Mueller, Principles of Surface Water Quality Modeling and Control

Dissolved oxygen content (DO) is a good indicator of the biochemical condition of water. For example, fish and other clean-water biota enjoy aquatic environment with high DO levels. Polluted streams with large loads of organic material (pollutions) are generally at low DO levels, which are unfavorable for clean-water species. To quantify the pollution load, measurement of BOD of water sample is often used.

Large Ultimate BOD values	highly polluted river
Low Ultimate BOD values	good quality water

BOD determination: diluting portions of a sample with oxygenated water and measuring the residual DO after a period of incubation (usually 5 days at 20°C). Then k (rate constant) is calculated.



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Weight of O_2 required per unit volume of the initial sample.

$$BOD \rightarrow \frac{dL}{dt} = -kL \quad \Rightarrow \quad L = L_{\infty} e^{-kt}$$

DO remaining: $C(t) = C_o - y(t)$

DO consumed

$$y(t) = L_{\infty}\left(1 - e^{-kt}\right)$$

$$C(t) = C_o - L_{\infty}\left(1 - e^{-kt}\right)$$

Estimation of k (rate = constant) (5 day test)

$$\frac{dL}{dt} = -kL \qquad L = L_{\infty} e^{-kt}$$

at

$$t = t_1 \qquad L_1 = L_{\infty} e^{-kt_1} \qquad (1)$$

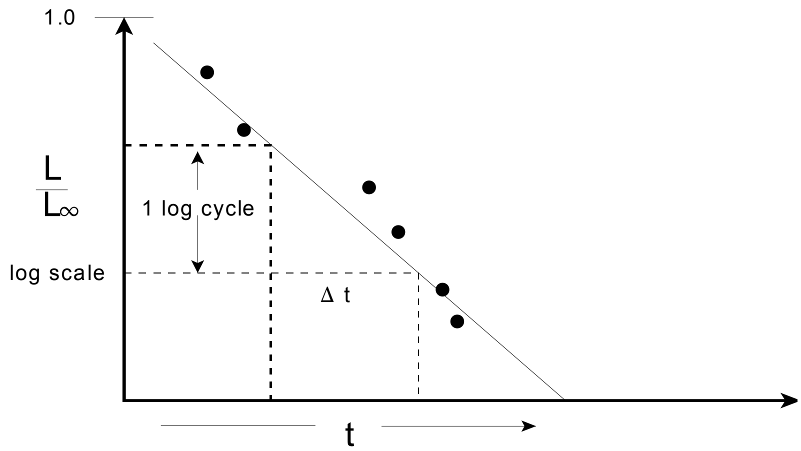
$$t = t_2 \qquad L_2 = L_{\infty} e^{-kt_2} \qquad (2)$$

$$\frac{(1)}{(2)} \quad \Rightarrow \quad \frac{L_1}{L_2} = e^{-k(t_1 - t_2)}$$

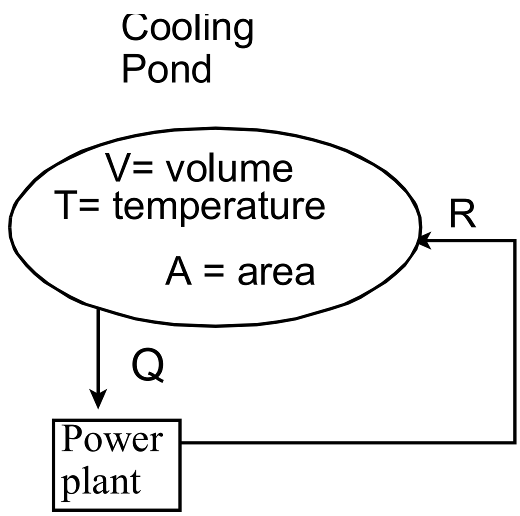
$$k = \frac{ln\, L_1 - ln\, L_2}{t_2 - t_1}$$

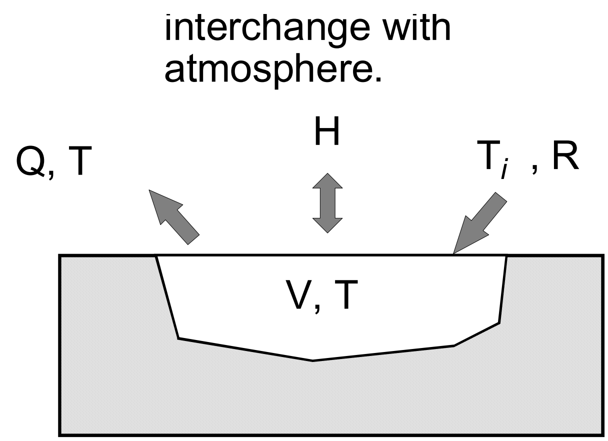
Graphical Method (A better way)

$$\ln\left(\frac{L}{L_{\infty}}\right) = -k\,t \qquad 2.3\log_{10}\left(\frac{L}{L_{\infty}}\right) = -kt \qquad k = \frac{2.3}{\Delta t}$$


1.0
L
L∞
log scale
1 log cycle
Δ t
t

Example (4) Power Plant Cooling Pond Design
(Ryan P.J. et al, 1974. ***WRR* 10 (5)**. p 930-939.





Definition: Kilocalorie (K cal): The energy required to raise the temperature of 1 kg of water by 1^{o}C. British thermal unit (B.T.U): the energy required to raise the temperature of 1 lb of water by 1^o F.

1 k cal = 3.968 B.T.U.

Thermal Energy (*E*) $$E = \int_V \rho \hat{c} T dV = \frac{[M]}{[L^3]} \cdot \frac{cal}{gm\ ^oC}\ ^oC [L^3]$$

where ρ is the density of water and $\hat{c}$ Is the specific heat of water which is the energy required to raise the temperature of a unit mass of material by one degree.

$$\hat{c} = \frac{1 cal}{gm^\circ C} = \frac{1 BTU}{lbm^\circ F}$$

Energy balance equation for the cooling pond is

$$\frac{d}{dt}(\rho \hat{c} T V) = \underbrace{\rho \hat{c} T_i R}_{\substack{\text{Energy}\\ \text{inflow}\\ \text{rate}}} \underbrace{- \rho Q T \hat{c}}_{\substack{\text{Energy}\\ \text{outflow}\\ \text{rate}}} \underbrace{+ H}_{\substack{\text{Netn heat}\\ \text{exchange}\\ \text{rate}}}$$

Steady flow: If we consider inflow to and outflow from the cooling pond is steady and assume the density of water change with little within the temperature range considered, we will

Let R = Q, $\boldsymbol{V}$ = constant, ρ = constant

The energy balance equation becomes

$$\frac{dT}{dt} = \frac{Q}{\boldsymbol{V}}\left(T_i - T\right) + \frac{H}{\rho \hat{c} \boldsymbol{V}}$$

Assumption: No seepage into or from groundwater, heat exchange occurs near the surface of the pond only and neglect heat conduction between the sounding soils.

Definition:

$\Phi_n = \frac{H}{A}$ = rate of net heat-transfer / unit area as a function of wind speed, water surface temp., air temp., and relative humidity.

The net heat transfer can also be evaluated using

$$\Phi_n = \Phi_r - \left(\Phi_{br} + \Phi_e + \Phi_c\right)$$

where φ_r = net incident radiation (long and short waves)

φ_e = surface heat flux by evaporation (latent head)

φ_c = surface heat flux by conduction (sensible heat)

φ_{br} = the surface back radiation

Formulas for each term are available but complicated. (see Ryan et al., 1974, or Thomann, p.602) Here, we will use a simple empirical relationship to determine the heat transfer. That is, we

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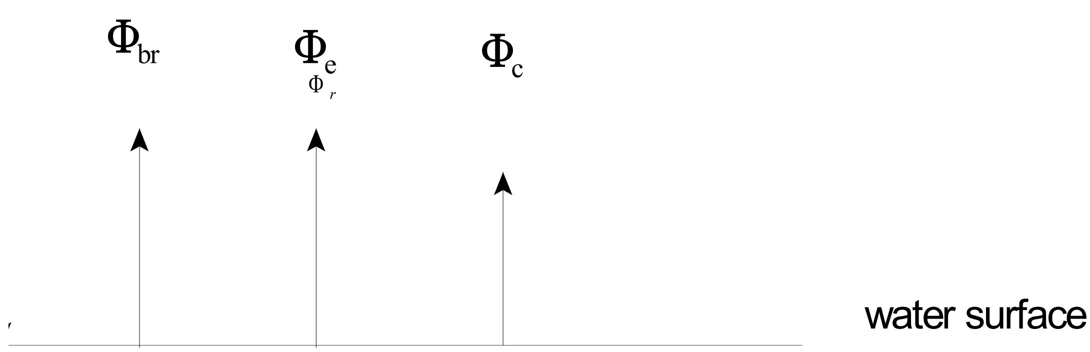
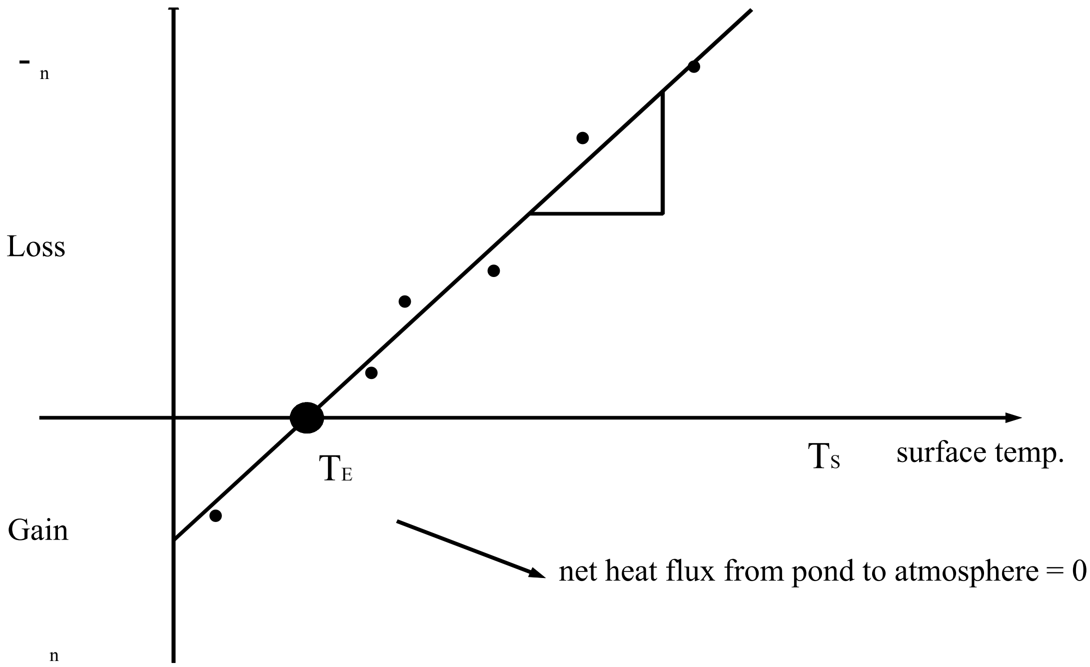




assume there exists a simple linear relationship between the net heat exchange rate and surface temperature of the water in the cooling pond:

$$\Phi_n = -K\left(T_S - T_E\right)$$

where T_E is the equilibrium temperature at which there is no net heat exchange between the atmosphere and the water. Its value varies with locality, solar radiation, wind speed, meteorological conditions and K is heat transfer coefficient, which has the unit of

$$= \frac{BTU}{ft^2 day\,°F} \qquad or \qquad \frac{cal}{m^2 sec\,°C}$$

If we assume that $T_S =$ T (i.e., a well-mixed system), then we have

$$\frac{dT}{dt} = \frac{Q}{\boldsymbol{V}}\left(T_i - T\right) - \frac{AK\left(T - T_E\right)}{\rho\,\hat{c}\boldsymbol{V}}$$

Now, we define water retention rate constant as $\frac{Q}{\boldsymbol{V}} = k_r$,[1/T] and the thermal rate constant as $\frac{AK}{\rho\,\hat{c}\boldsymbol{V}} = k_T$,[1/T]. The energy balance equation takes a new form:

$$\frac{dT}{dt} = k_r\left(T_i - T\right) - k_T\left(T - T_E\right)$$

Consider a steady state energy system:

$$\frac{dT}{dt} = 0 \quad T \to \infty\,; \quad \text{at} \quad \text{which} \;\; T = T_\infty$$

Assuming that Ti is constant, we have

$$k_r\left(T_i - T_\infty\right) = k_T\left(T_\infty - T_E\right)$$

$$k_r\left[\left(T_i - T_E\right) - \left(T_\infty - T_E\right)\right] = k_T\left(T_\infty - T_E\right)$$

$$\frac{T_\infty - T_E}{T_i - T_E} = \frac{k_r}{k_r + k_T} = \frac{1}{1+r}$$

where $r = \dfrac{k_T}{k_r}$, which is a characteristics of a cooling pond. k_r and k_T can be estimated from temperature data of the site.

Again, whenever a lumped parameter model is applied to a problem, which is not fully well mixed, the state variable in the model represents only the value of the state variable averaged over the entire system–not a point observation of the state variable in the system.

Other applications: Geothermal reservoirs, groundwater remediation, DNPLs estiamtion, etc.

Analytical Solutions to the Lumped Parameter Models:

Water Quality in Lakes:

$$\frac{dC}{dt} + C\left(\frac{R}{V}\right) = C_i\left(\frac{R}{V}\right) + S$$

$$\frac{dC}{dt} + k_r C = k_r C - \underbrace{k\,C}_{\substack{\text{1stn Order} \\ \text{Decay}}}$$

or

$$\frac{dC}{dt} + \left(k_r + k\right)C = k_r C_i$$

This equation is a first-order linear differential equation,

(a) Steady State

$$\frac{dC}{dt} = 0 \quad \rightarrow \quad C_i \text{ constant} \quad \text{or} \quad t \rightarrow \infty$$

$$\left(k_r + k\right)C = k_r\,C_i$$

$$C = \left(\frac{k_r}{k_r + k}\right)C_i$$

Example:

V / R = 10 days (retention time) = $1 / k_r$

$$\therefore k_r = 0.1\,day^{-1}$$

$$k = 1\,day^{-1} \qquad \text{(rate constant)}$$

$$C = \frac{k_r}{k + k_r}\,C_i$$

$$= \frac{0.1 C_i}{1 + 0.1} = 0.09\,C_i$$

This implies that the contaminant decays substantially in this reservoir.

If $k = 0$, (i.e., conservative chemical)

$$C = \frac{0.1}{0+0.1} C_i = 1 C_i$$

The result shows that the concentration of α in the reservoir is equal to the inflow concentration as $t \to \infty$ (i.e., at equilibrium stage).

Transient Cases:

Now let's examine the transient situation (before the system reaches equilibrium stage). In this case, the response of the system or reservoir depends on the type of input.

1) Impulse Input

A mass of contaminant, M, is suddenly discharged into a lake at $t = 0$.

$$\rho Q C_i = M\delta(t) \qquad C_i = \frac{M\delta(t)}{\rho Q}$$

where $\delta(t)$ is the Dirac delta function, [1/T]. Therefore, the concentration is

$$C_i = \frac{[M_\alpha]\left[\frac{1}{T}\right]}{\left[\frac{M_w}{L^3}\right]\left[\frac{L^3}{T}\right]} = \left[\frac{M_\alpha}{M_w}\right]$$

$$Q = \left[\frac{L^3}{T}\right]$$

$$\rho = \left[\frac{M}{L^3}\right]$$

Mathematically, the impulse function can be rewritten as

$$\int_{-0}^{+0} \delta(t)\,dt = 1 \quad \text{and} \quad \delta(t) = 0 \quad t \neq 0$$

Then the mass balance equation becomes:

$$\frac{dC}{dt} + k_e C = \frac{Q}{V} C_i = \frac{Q}{V} \cdot \frac{M\delta(t)}{\rho\, Q} = \frac{M\delta(t)}{V\rho}$$

We will let

$$k_e = \left(\frac{Q}{V} + k\right) = (k_r + k)$$

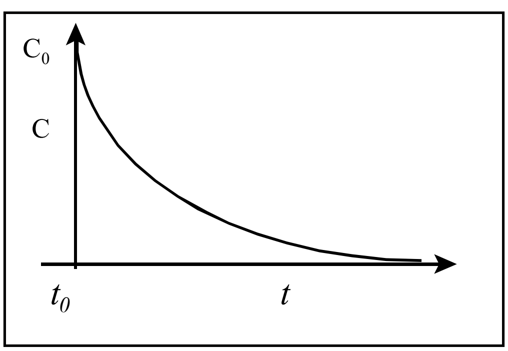
in which k_e^{-1} denotes the reservoir chemical response time. Then, we have

$$\frac{dC}{dt} + k_e C = \frac{M\delta(t)}{V\rho}$$

Notice the dimension of each term in the equation is [1/T]

Consider the case where $t \neq 0$. Then, δ=0 and the chemical mass balance equation becomes

$$\frac{dC}{dt} + k_e C = 0$$



The solution to the equation is

$$C = C_o e^{-k_e t},$$

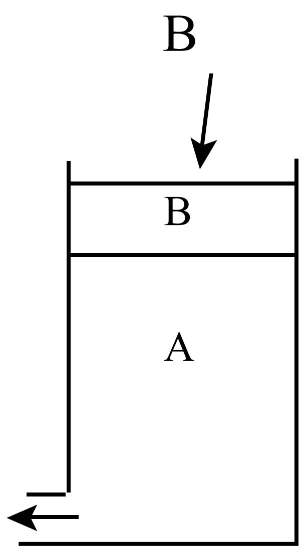
where C_o = concentration at $t = t_o$. Or we can write the solute as

$$C = C_o e^{-(k_r + k)t}$$

Let's assume $k = 0$ (i.e., the tracer is nonreactive). We now have

$$C = C_o e^{-k_r t}$$

This means that the concentration of α chemical in the reservoir and the outflow will decrease exponentially as time progresses. This decrease in concentration is attributed to mixing or dilution resulting from the inflow of fresh water after the impulse input. To allow the reservoir to return to the initial concentration, say $C_o = 0$, according the solution, t must approach infinity. Notice the distinction between the retention time (t_r) and this t. While it will take a finite time, t_r, to fill up the reservoir, why does it have to take an infinite amount of time to completely flush out the reservoir? We consider the following two cases.

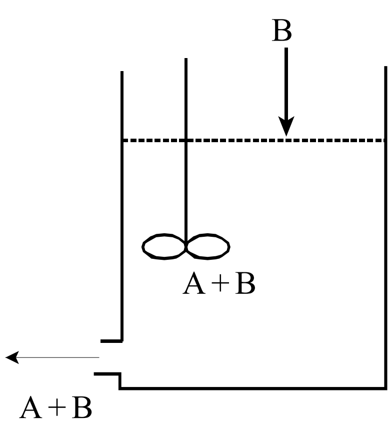


Case 1. No mixing

In this case, the time to drain fluid A completely from the reservoir or the time needed to fill the reservoir with fluid B is the retention time,

$$t_r = \frac{1}{k_r} = \frac{V}{Q}$$

Case 2: Mixing is involved. The time to completely replace fluid A by fluid B will be infinite.



Now consider when t =0, and the initial concentration of α in the reservoir is $C_o = 0$.

$$\frac{dC}{dt} + k_e C = \frac{M}{\rho \boldsymbol{n} \boldsymbol{V}} \delta(t)$$

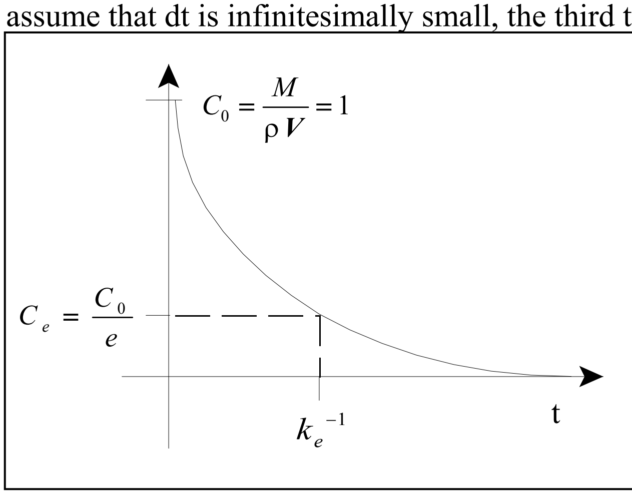
Integrate the equation around the time origin.

$$\int_{0-}^{0+} \left(\frac{dC}{dt} + k_e C \right) dt = \int \frac{M}{\rho \boldsymbol{V}} \delta(t)\, dt$$

$$\int_{0-}^{0+} dC + k_e \int_{0-}^{0+} C\, dt = \frac{M}{\rho \boldsymbol{V}} \int_{0-}^{0+} \delta(t)\, dt$$

$$C(0^+) - C(0^-) + k_e \int_{0-}^{0+} C\, dt = \frac{M}{\rho \boldsymbol{V}}$$

The concentration at $t=0^-$ is zero since the initial condition is assumed to be zero. Further, we assume that dt is infinitesimally small, the third term is then zero. Therefore, for t=0.



$$C_o = \frac{M}{\rho \boldsymbol{V}}$$

and for $t > 0$,

$$C = \frac{M}{\rho \boldsymbol{V}} e^{-k_e t}$$

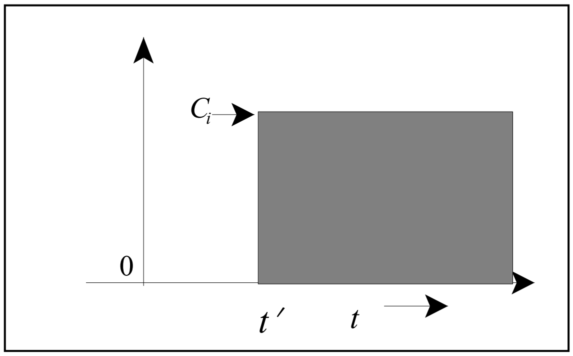
If $\frac{M}{\rho \boldsymbol{V}} = 1$, the input is called the unit impulse input.

$$C_e = \frac{M}{\rho \boldsymbol{V}} e^{-k_e \left(\frac{1}{k_e} \right)} = \frac{M}{\rho \boldsymbol{V}} e^{-1} = \frac{C_1}{e}$$

C_e = concentration at the chemical response time, which is defined as t_e and is equal to $\frac{1}{k_e}$

2). Step Input.

This input aims to represent a sudden discharge of a constant, continuous concentration, C_i from a source to the reservoir. Mathematically, the step input is defined as



$$C = 0 \text{ at } \quad t < t$$

$$C = C_i \text{ at } t \geq t'$$

The governing equation is

$$\frac{dC}{dt} + \left(k_r + k\right)C = k_r C_i$$

where C_i = constant. Let $k_r + k = k_e$, we have

$$\frac{dC}{dt} + k_e C = k_r C_i$$

To solve this equation for the step input, Recall

$$y' + f\left(x\right) y = r\left(x\right) \neq 0$$

and the magic formula $\quad y\left(x\right) = e^{-h}\left[\int e^h r\, dx + A\right]$

where $\quad h = \int f\left(x\right) dx$

$$f(x) \Rightarrow k_e \qquad h = \int k_e\, dt = k_e t$$
$$r(x) \Rightarrow k_r C_i$$

Then, the general solution becomes

$$C\left(t\right) = e^{-k_e t}\left[\int e^{k_e t} k_r C_i\, dt + A\right]$$

$$= e^{-k_e t}\left[\frac{k_r C_i}{k_e} \cdot e^{k_e t} + A\right]$$

To derive the unknown constant, A, in the solution, an initial condition must be used.

If $t = t_1' = 0, \quad C_o = 0$

$$0 = \frac{k_r C_i}{k_e} + A e^{-k_e t}$$

the constant is

$$A = -\frac{k_r C_i}{k_e}$$

Substituting the constant to the general solution,

$$C(t) = \frac{k_r C_i}{k_e} - \frac{k_r}{k_e} C_i \cdot e^{-k_e t}$$

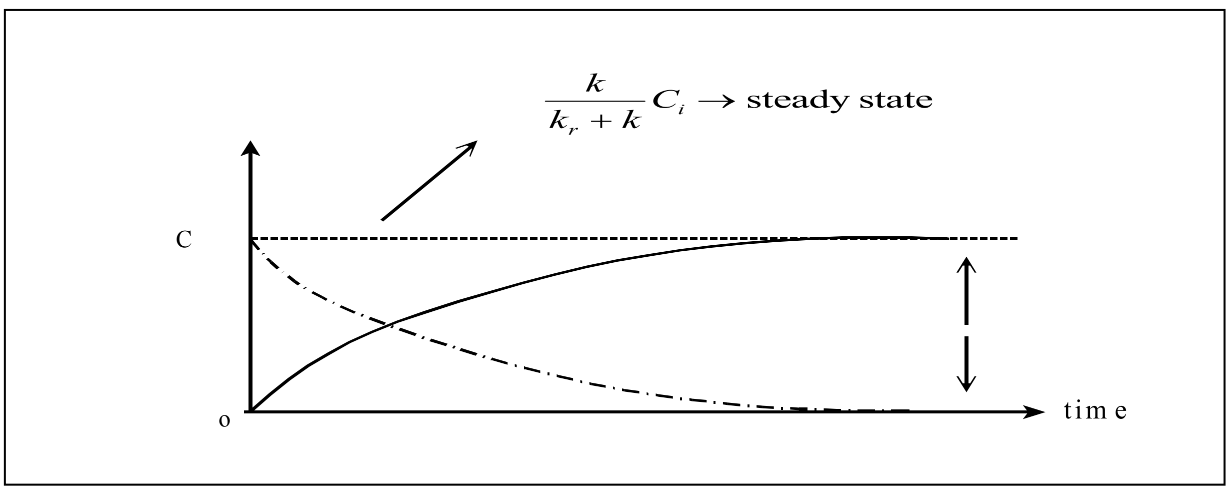
The final particular solution takes the form,

$$C(t) = \frac{k_r}{k_e} C_i \left(1 - e^{-k_e t}\right)$$

Or

$$\frac{C(t)}{C_i} = \frac{k_r}{k_r + k}\left(1 - e^{-k_e t}\right)$$

The graph of the solution is given in the figure below



This solution is similar to:

$L = L_\infty \left(1 - e^{-kt}\right)$ BOD

Now consider if at $t = t_1 = 0$, $C = C_0 \neq 0$.

$$C_o = \frac{k_r}{k_e} C_i + A$$

The constant associated with the initial condition is

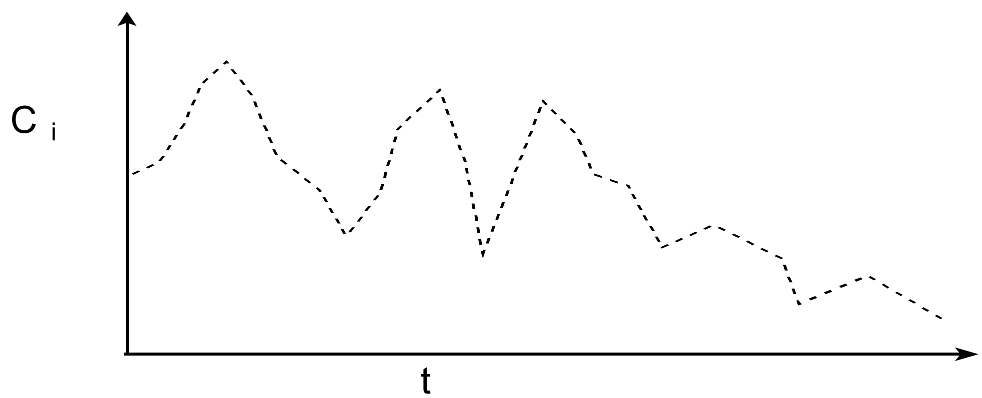
$$A = C_o - \frac{k_r}{k_e} C_i$$

The particular solution takes the form

$$C(t) = \frac{C_i k_r}{k_r + k}\left(1 - e^{-k_e t}\right) + C_o e^{-k_e t}$$

The solution consists of two parts: 1) the first term, which represents the effect of inflow concentration due to mixing and chemical reaction in the reservoir and 2) the second term, which denotes the change in initial concentration due to mixing and chemical reaction.

Arbitrary Input (the **most common form in nature)**



The governing equation is

$$\frac{dC}{dt} + k_e C = k_r C_i(t)$$

No exact math function for C_i.

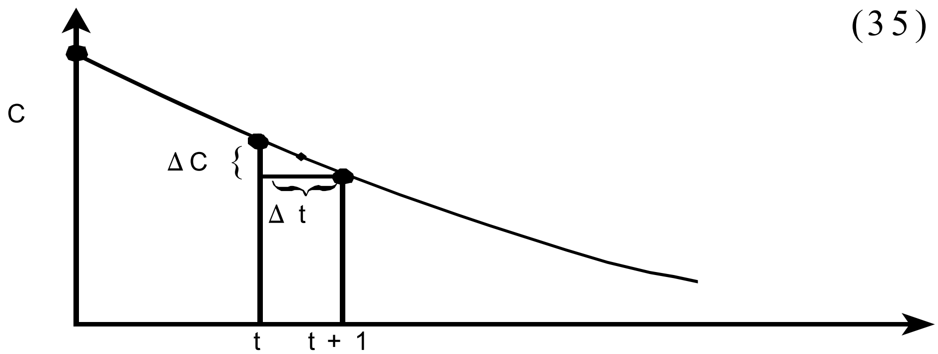
Approaches:

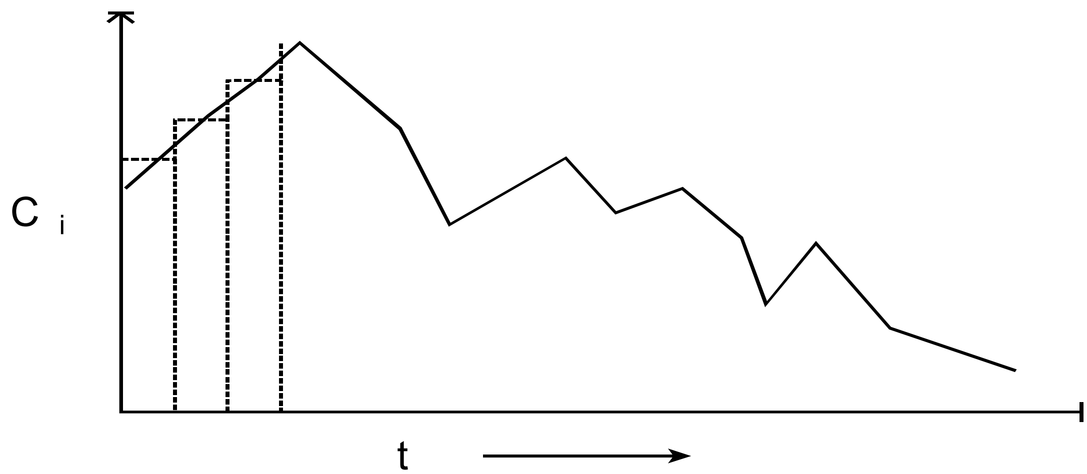
(1) Numerical Solution (Finite Difference):

Numerical approximation:

$$\frac{dC}{dt} \approx \frac{\Delta C}{\Delta t} = \frac{C^{t+1} - C^{t}}{\Delta t} \qquad \textit{Forward Finite Difference}$$

(3 5)





Therefore (1) becomes:

$$\frac{dC}{dt} \approx \frac{\Delta C}{\Delta t} = \frac{C^{t+1} - C^{t}}{\Delta t},$$

where: Δt = the average concentration between $t + 1$ and t, C^{t+1} = concentration at time $t = \Delta t$, and is the unknown to be solved, and C^{t} = concentration at time t. Subsequently, the finite difference solution is

$$C^{t+\Delta t} = \frac{1}{\left(1+\frac{\Delta t k_e}{2}\right)}\left[C^{t}\left(1-\frac{k_e \Delta t}{2} + k_r\, \Delta t\, C_i^{t}\right)\right]$$

C_i^t can be obtained by discretizing the input concentration record.

(2) Analytical Approach:

take advantage of the solution for step inputs

1. Descretize the inflow concentration record into slugs.
2. Treat each step (or slug) as a step input.

$$C(t) = \frac{k_r}{k_e} C_i \left(1 - e^{-k_e t}\right) + C_o e^{-k_e t}$$

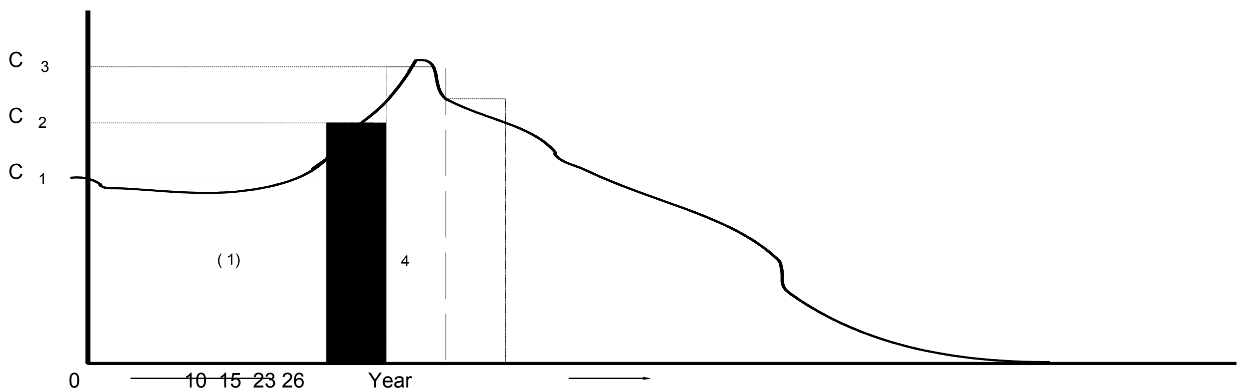
where C_o = initial concentration at that time step

C_i = inflow concentration at that time step

C = outflow concentration at that time step

3. Use *C* as the initial concentration for the next time step.
4. Repeat procedures (2) & (3).

Example



(1) Treat the variable input as consecutive step slugs.

Solution for time period #1 (10 Years):

$$C(t) = \frac{k_r}{k_e} C_i \left(1 - e^{-k_e t}\right) + C_o e^{-k_e t}$$

At the end of the 10th year, the outflow concentration becomes:

$$C_{10} = \frac{k_r}{k_e} C_{i_o} \left(1 - e^{-k_e(10)}\right) + C_o e^{-k_e(10)}$$

Use this concentration as the initial concentration for the second (2) period:

$$C_{15} = \frac{k_r}{k_e} \left[C_{i_{10}}\right]^* \left(1 - e^{-k_e(5)}\right) + C_{10} e^{-k_e(5)}$$

Before we proceed to the harmonic input, we review some fundamentals of complex variable.

Complex variable

$$z = \underbrace{x}_{\text{real}} + \underbrace{iy}_{\substack{\text{imaginary} \\ \text{nparts}}}$$

z plotted on a complex plane.

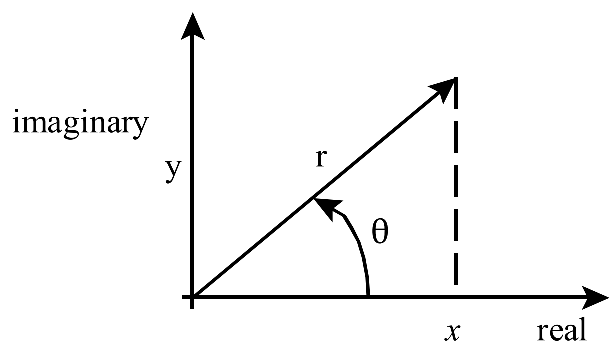
$$x = r\cos\theta, \quad y = r\sin\theta$$

$$\therefore z = r\left(\cos\theta + i\sin\theta\right)$$

Euler's formula:

$$z = re^{i\theta} \qquad \therefore \quad e^{i\theta} = \cos\theta + i\sin\theta$$

$$\theta = \tan^{-1}\left(\frac{y}{x}\right)$$



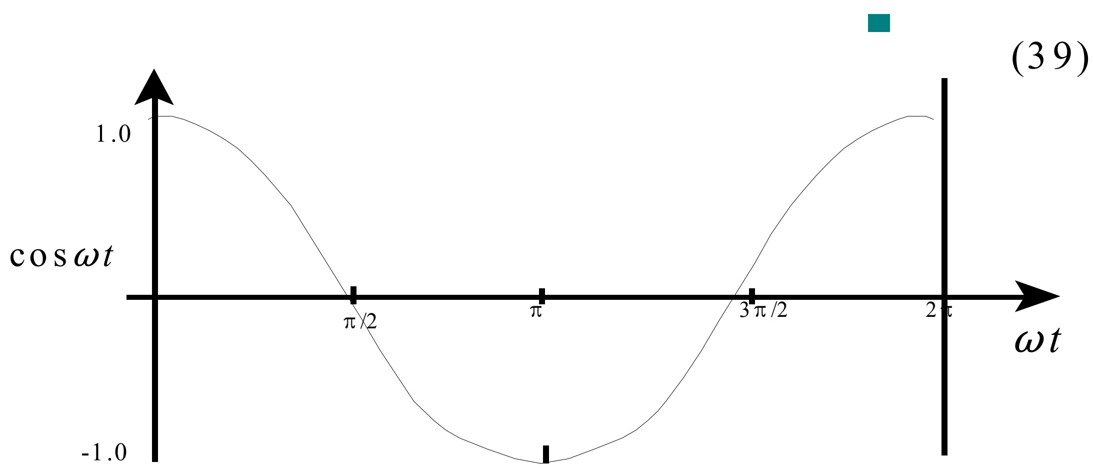
Harmonic Input (Periodic Input):

Example: Processes that are subject to diurnal variation (e.g., DO in water due to photosynthesis).

Let's assume Input Form:

$$C_i(t) = a\cos\omega t$$

where a = amplitude [M/L^3], ω = frequency [1/T]



Assume $C(0) = 0$

Mass Balance Equation:

$$\frac{dC}{dt} + k_e C = k_r C_i(t) = k_r a\cos\omega t \qquad \text{— (1)}$$

$$= k_r a e^{i\omega t} \qquad \text{use Euler's formula.}$$

Solution:

Assume that the solution is in this form:

$$C(t) = \phi e^{i\omega t} \qquad \text{— (2)}$$

Substitute (2) into (1) to obtain

$$i\omega e^{i\omega t} + k_e \phi e^{i\omega t} = k_r a e^{i\omega t}$$

$$i\omega\phi + k_e\phi = k_r a$$

$$\phi = \frac{a k_r}{i\omega + k_e} \qquad \text{-----(3)}$$

Then, substitute (3) into (2) to yield

$$C(t) = \frac{a k_r}{i\omega + k_e} e^{i\omega t}$$

Now, use $z = k_e + i\omega = re^{i\theta}$

where $r = \left(k_e^2 + \omega^2\right)^{1/2}$

$$\theta = \tan^{-1}\left(\omega / k_e\right)$$

Final solution takes the form:

$$C(t) = \frac{a k_r}{\left(k_e^2 + \omega^2\right)^{1/2}} e^{i(\omega t - \theta)} = \frac{a k_r}{\left(k_e^2 + \omega^2\right)^{1/2}} \cos\left(\omega t - \theta\right)$$

or

$$C(t) = a A_m \cos\left(\omega t - \theta\right)$$

where $A_m = \dfrac{k_r}{\left(k_e^2 + \omega^2\right)^{1/2}}$

Attenuation on amplitude (Amplitude effect)

$$\theta = \tan^{-1}\left(\frac{\omega}{k_e}\right)$$

Delay on phase (Phase lag) (Phase effect)

$$0 \le \theta \le \frac{\pi}{2}$$

Based on analysis of this simple model, we can conclude that input of high frequencies (noise or short-term temporal variations) are most likely attenuated and delayed in the output. On the other hand, input of low frequencies (long-term temporal variations) are likely to be preserved in a well-mixed system.

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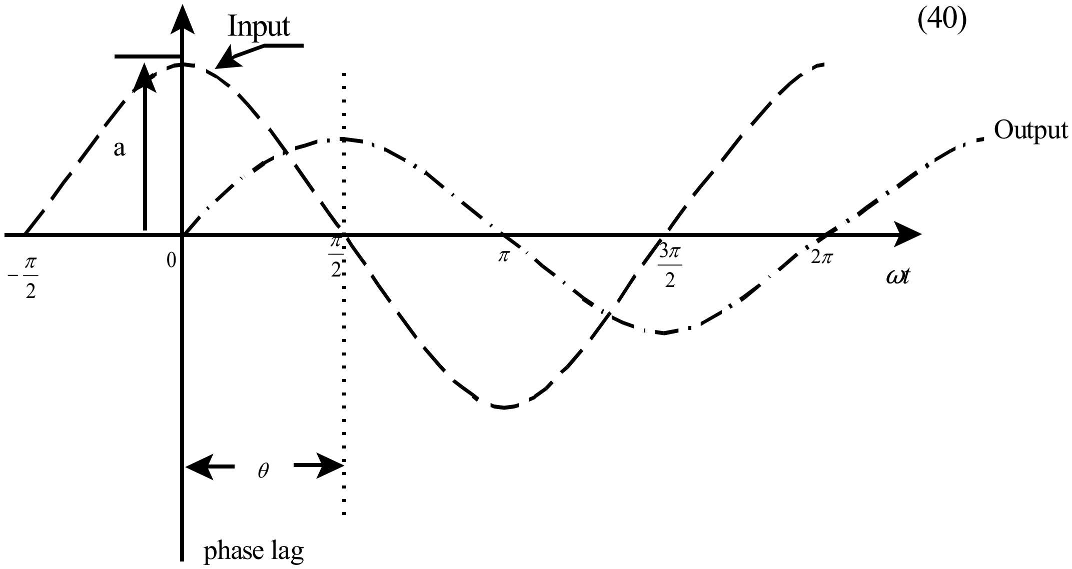
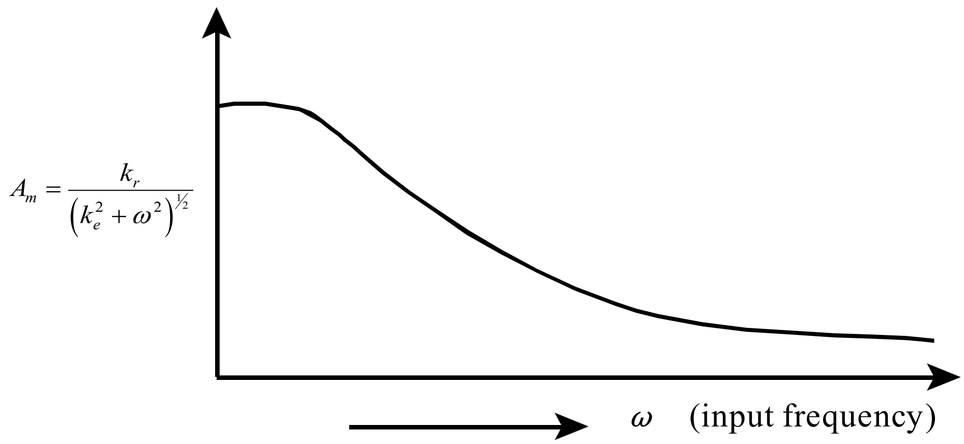
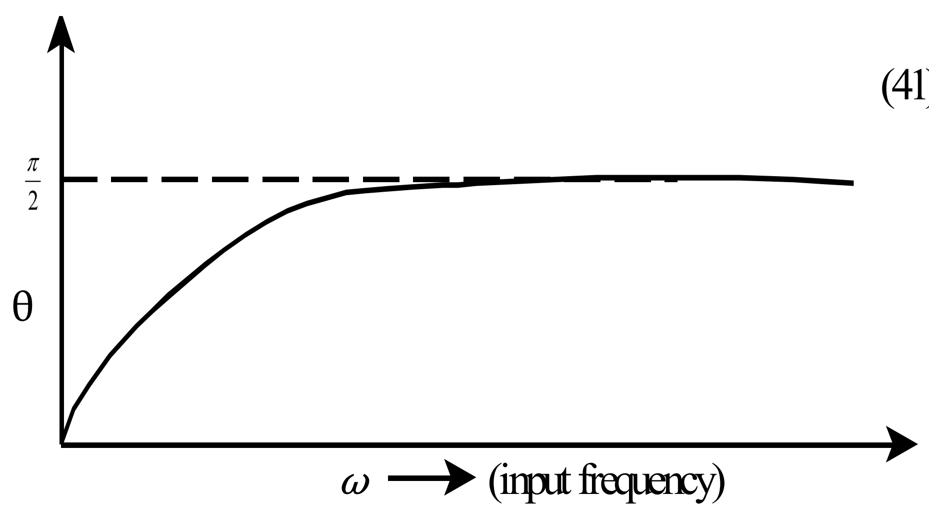

Input
Output
a
$-\frac{\pi}{2}$
0
$\frac{\pi}{2}$
π
$\frac{3\pi}{2}$
2π
ωt
θ
phase lag



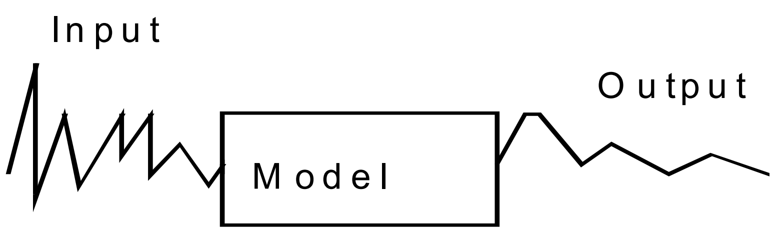
* Attenuation and phase effects are significant for large ω frequency input, and depend on:

k_r = retention characteristics of the system
k = rate constant of the chemical
ω = input frequency

(41)



Parameter Estimation

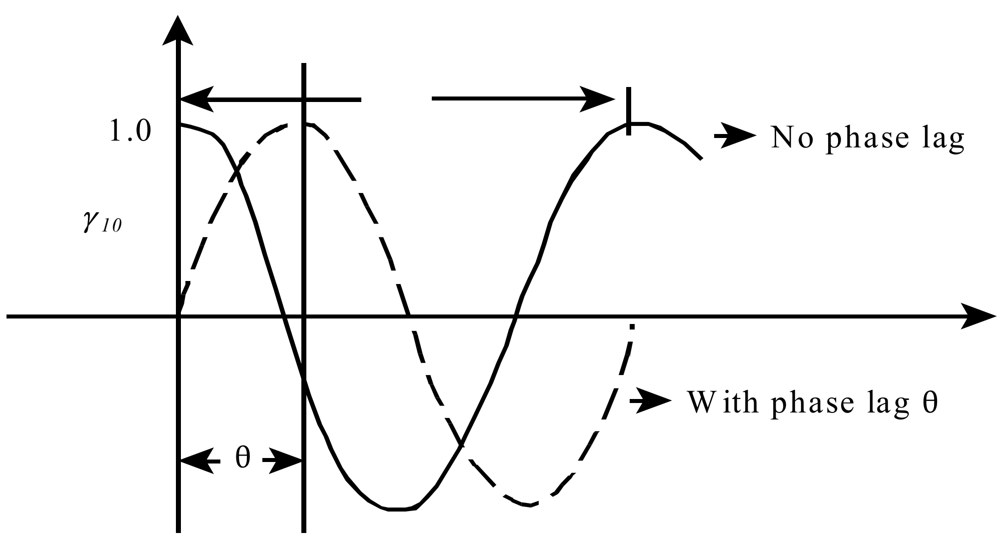


Parameter estimation is a technique to estimate the parameter values in the lumped parameter, using observed input and output.

Real data ~Noise~

Cross-correlation Analysis ⟹ Calculate the correlation of the input and the output series at different lags.

(43)



$$\theta = \tan^{-1}\left(\frac{\omega}{k_e}\right)$$

$\Rightarrow$ *Autocorrelation* $\Rightarrow$ ω.

k_e is predetermined.

$$A_m = \frac{k_r}{\left(k_e^2 + \omega^2\right)^{1/2}} \qquad k_r \to k\ .$$

Comments:

The most frequent misuse of the lumped parameter model is the failure of recognizing the difference between a spatial point observation of a system and the well-mixed assumption behind the lumped model. That is, the results of a lumped parameter model are often compared with a single spatial point observation of a system. Likewise, a single spatial point observation often has been used to estimate the parameter value of a lumped parameter model. Do you have to be a rocket scientist to understand this inconsistency (do not compare apples to oranges!–common sense)? No wonder that they cannot solve the problem. On the other hand, most of you unfortunately believe in them because you are scared by their Ph.D. (Pile higher and Deeper) degree in some special field and fancy jargons and their predatory nature. Wake up! God gives you common sense to survive and you are at least as smart as those who have alligator skins and dare to lie (they know they do not know what true is!). Believe in yourself, not your professors nor those so-called scientists and politicians.

To meet the well-mixed assumption, one should take as many point samples at different location of the system as possible and then average them to obtain the average response of the system. Otherwise, for example, determine the chemical response time of the system, average the observed concentration data over the response time, and then compare them with the model results. This is approach relies on the assumption that at the response time, the system becomes relatively well mixed.

"A Water Quality Model of "Chlorides" in Great Lakes". O'Connor and Mueller, San. Engineering Division ASCE, Vol. 96 (SA4) 955-975, 1970.

Combination of Well-mixed systems.

Well-mixed assumption

Time interval - 1yr. Time scale is large enough to meet the well-mixed assumption.

Inflow: Basin runoff
Precipitation on lake

Outflow: Evaporation from lake
Discharge to other lakes, ocean

Pollutant Sources:

1. Natural Background Concentrations - initial concentrations
2. Municipal - Chlorides introduced by human and domestic wastes and various commercial usages.
3. Industrial -

4. Road Salt (de-icing salt)
5. Other Sources (fudge factor)

Conclusions:

1. In spite of incomplete data on various sources, agreement between the calculated and observed values is reasonably good.

2. The model quantitizes the magnitude of various sources of potential pollutants, so that their relative importance maybe assessed.

3. Effects of imposing controls on waste load inputs.

Acid Rain Project.

Well-mixed systems may be used as a basis for a preliminary analysis.