LECTURE

MODELLING THE MARINE ENVIRONMENT

Lecturer: Prof. Nguyen Ky Phung

MSc. Dang Thi Thanh Le

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Lecture 7

PROCESS OF SUBSTANCE TRANSMISSION

Lecturer: Prof. Nguyen Ky Phung
MSc. Dang Thi Thanh Le

Lecture 7B

SYSTEM OF REACTOR

Lecturer: Professor. TS. Nguyen Ky Phung
Ms. Dang Thi Thanh Le

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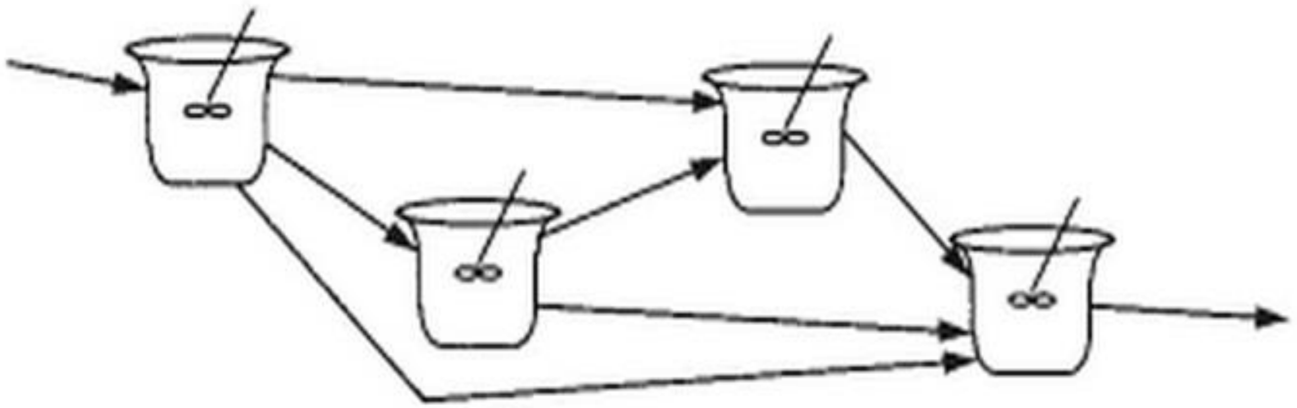
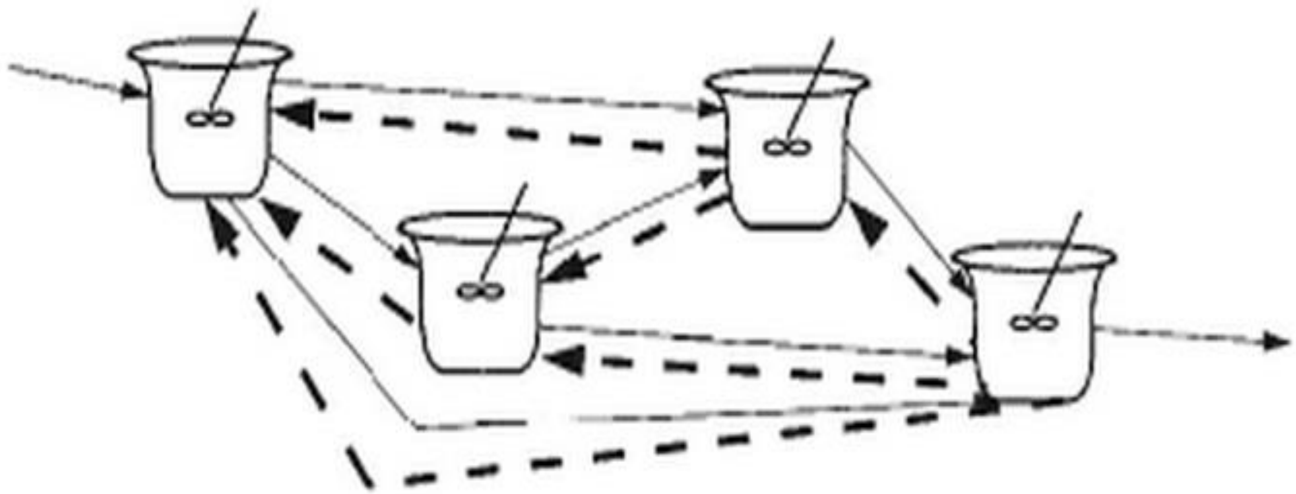


(a) **Moving Impact System**



(b) **Reponses Impact System**

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Moving Impact System

SOLUTION FOR THE STABLE STATE

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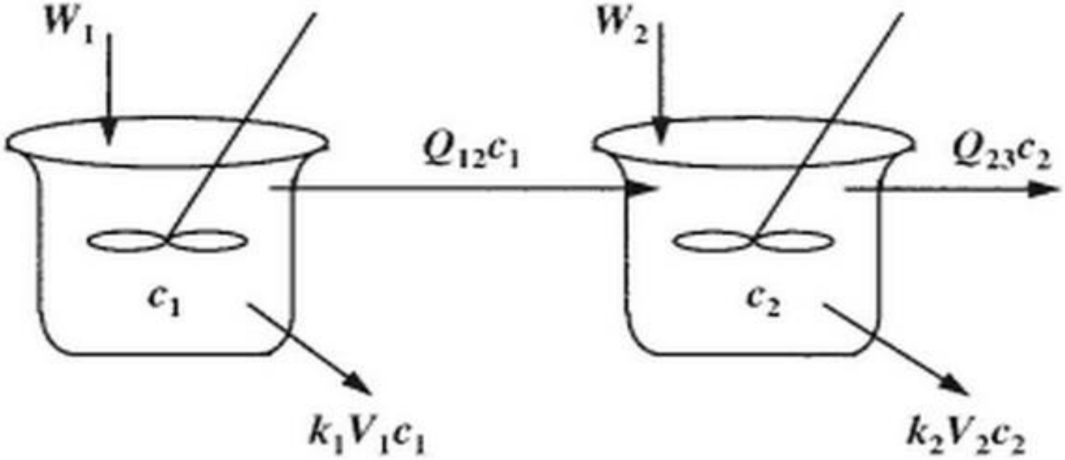
A simple application is to simulate a chain of interconnected lakes using short river sections. In this case, we consider a simple system of two lakes as described:



Mass balance for these reactors can be written:

Lake 1 $$V_1 \frac{dC_1}{dt} = W_1 + Q_{01}C_0 - Q_{12}C_1 - k_1V_1C_1 \quad (1)$$

Lake 2 $$V_2 \frac{dC_2}{dt} = W_2 + Q_{12}C_1 - Q_{23}C_2 - k_2V_2C_2 \quad (2)$$

SOLUTION FOR THE STABLE STATE

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At steady – state:

$$a_{11}C_1 = W_1 \quad (3)$$

$$-a_{21}C_1 + a_{22}C_2 = W_2 \quad (4)$$

where

$$a_{11} = Q_{12} + k_1V_1 \qquad a_{21} = Q_{12} \qquad a_{22} = Q_{23} + k_2V_2$$

Solution

Lake 1 $$C_1 = \frac{1}{a_{11}}W_1 = \frac{1}{Q_{12} + k_1V_1}W_1 \quad (5)$$

Lake 2 $$C_2 = \frac{W_2 + a_{21}C_1}{a_{22}} = \frac{1}{Q_{23} + k_2V_2}W_2 + \frac{Q_{12}}{Q_{23} + k_2V_2}\,\frac{1}{Q_{12} + k_1V_1}W_1 \quad (6)$$

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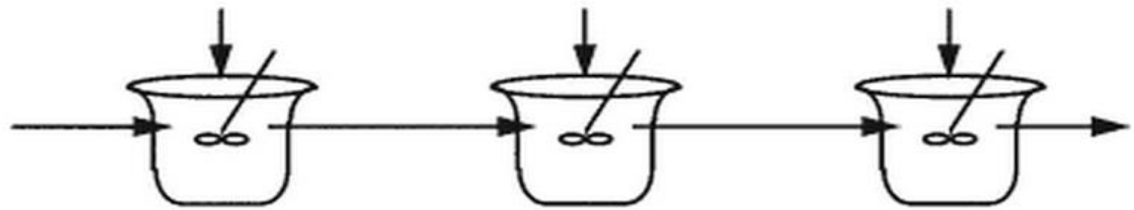
Example 1. Suppose that three lakes are connected in series. The pollutant settles at a rate of 10 m/yr.

(a) Determining concentrations in the steady- state of each reactor

(b) Determining how much the concentration in the third reactor to the loading of the second reactor.



		Lake 1		Lake2		Lake 3	
Volume, 10^6 m^3		2		4		3	
Depth, m		3		7		3	
Surface area, 10^6 m^2		0.667		0.571		1.000	
Loading, kg/yr		2000		4000		1000	
Flow, 10^6 m^3/yr	1.0		1.0		1.0		1.0

Solution

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(a) The concentration of the lakes is determined as follows:

$$C_1 = \frac{W_1}{Q_{12} + vA_1} = \frac{2\times 10^9}{1.0\times 10^6 + \left(10\times 0.667\times 10^6\right)} = 260.76\mu g L^{-1}$$

$$C_2 = \frac{W_2}{Q_{23} + vA_2} + \frac{Q_{12}C_1}{Q_{23} + vA_2} = \frac{4\times 10^9}{1.0\times 10^6 + \left(10\times 0.571\times 10^6\right)} + \frac{1.0\times 10^6\left(270.76\right)}{1.0\times 10^6 + \left(10\times 0.571\times 10^6\right)}$$

$$= 596.13 + 38.86 = 634.99\mu g L^{-1}$$

$$C_3 = \frac{W_3}{Q_{34} + vA_3} + \frac{Q_{23}C_2}{Q_{34} + vA_3} = \frac{1\times 10^9}{1.0\times 10^6 + \left(10\times 1\times 10^6\right)} + \frac{1.0\times 10^6\left(634.99\right)}{1.0\times 10^6 + \left(10\times 1\times 10^6\right)}$$

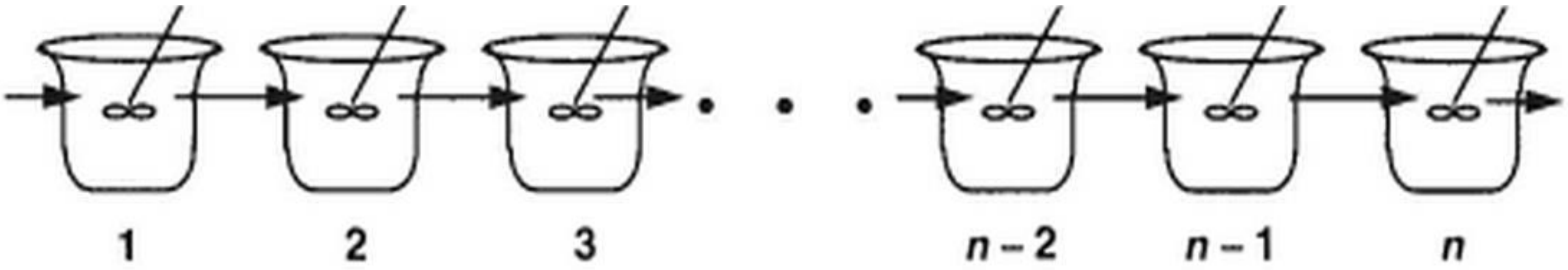
$$= 148.64\mu g L^{-1}$$

(b) As the solution to C2 above we notice., 596.13μgL^{-1} of C_2 due to load into lake 2 (W_2), whereas 38.86μgL^{-1} it is due to loading into lake 1. Therefore, the effect of Lake 2 on Lake 3 can be calculated as follows:

$$\frac{1.0\times 10^6\left(596.13\right)}{1.0\times 10^6 + \left(10\times 1\times 10^6\right)} = 54.19\mu g L^{-1}$$

SOLUTION FOR THE STABLE STATE

A special case for the system of well-mixed lakes is when the volume and flow of the lakes are the same



Cascade model

The solution of the lakes is simplified as follows

Lake 1 $$C_1 = \frac{Q}{Q+kV} C_0$$

Lake 2 $$C_2 = \frac{Q}{Q+kV} C_1 = \frac{Q}{Q+kV} \frac{Q}{Q+kV} C_0$$

Lake n $$C_n = \left(\frac{Q}{Q+kV} \right)^n C_0$$

SOLUTION FOR THE UNSTABLE STATE

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Equations (1) and (2) in case W = 0 are written as follows:

Lake 1 $$\frac{dC_1}{dt} = -\lambda_{11} C_1 \qquad (7)$$

Lake 2 $$\frac{dC_2}{dt} = \lambda_{21} C_1 - \lambda_{22} C_2 \qquad (8)$$

Where $\lambda_{11} = \frac{Q_{12}}{V_1} + k_1$ $\quad \lambda_{21} = \frac{Q_{12}}{V_1}$ $\quad \lambda_{22} = \frac{Q_{23}}{V_2} + k_2$

At t = 0: $C_1 = C_{10}$ and $C_2 = C_{20}$, We have the following solution.:

Lake 1 $$C_1 = C_{10} e^{-\lambda_{11} t} \qquad (9)$$

Lake 2 $$C_2 = C_{20} e^{-\lambda_{22} t} + \frac{\lambda_{21} C_{10}}{\lambda_{22} - \lambda_{11}} \left(e^{-\lambda_{11} t} - e^{-\lambda_{22} t} \right) \qquad (10)$$

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SOLUTION FOR THE UNSTABLE STATE

To find a general solution to the system of lakes, Di Toro (1972) developed the following relationship:

Lake 1 $C_1(t,\lambda_{11}) = C_{10}e^{-\lambda_{11}t}$

Lake2 $C_2(t,\lambda_{11},\lambda_{22}) = \frac{\lambda_{21}}{\lambda_{22}-\lambda_{11}}\left[C_1(t,\lambda_{11}) - C_1(t,\lambda_{22})\right]$

Lake 3 $C_3(t,\lambda_{11},\lambda_{22},\lambda_{33}) = \frac{\lambda_{32}}{\lambda_{33}-\lambda_{22}}\left[C_2(t,\lambda_{11},\lambda_{22}) - C_1(t,\lambda_{11},\lambda_{33})\right]$

Lake 4 $C_4(t,\lambda_{11},\lambda_{22},\lambda_{33},\lambda_{44}) = \frac{\lambda_{43}}{\lambda_{44}-\lambda_{33}}\left[C_3(t,\lambda_{11},\lambda_{22},\lambda_{33}) - C_1(t,\lambda_{11},\lambda_{22},\lambda_{44})\right]$

Lake n $C_n(t,\lambda_{11},...,\lambda_{n,n}) = \frac{\lambda_{n,n-1}}{\lambda_{n,n}-\lambda_{n-1,n-1}}\left[C_{n-1}(t,\lambda_{11},...,\lambda_{n-2,n-2},\lambda_{n-1,n-1}) - C_{n-1}(t,\lambda_{11},....,\lambda_{n-2,n-2},\lambda_{n,n})\right]$

The general form of this factored version is

$$C_n(t,\lambda_{11},...,\lambda_{n-1,n-1},\lambda_{n,n}) = \prod_{j=1}^{n-1}\lambda_{j+1,j}\sum_{i=1}^{n}\frac{C_1(t,\lambda_{i,i})}{\prod_{j=1(j\neq i)}^{n}(\lambda_{j,j}-\lambda_{i,i})}$$

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Reponses Impact System

REPONSES IMPACT SYSTEM

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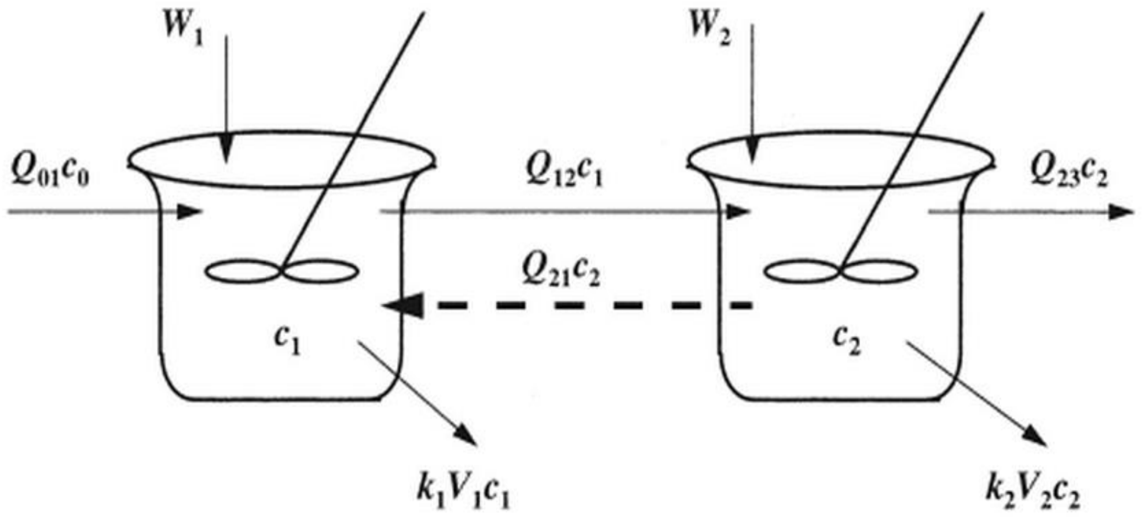
In this case, we consider a simple system of two lakes as described:



Mass balances for two CSTRs with feedback can be written

Lake 1 $$V_1 \frac{dC_1}{dt} = W_1 + Q_{01}C_0 - Q_{12}C_1 - k_1V_1C_1 + Q_{21}C_2 \quad (11)$$

Lake 2 $$V_2 \frac{dC_2}{dt} = W_2 + Q_{12}C_1 - Q_{21}C_2 - Q_{23}C_2 - k_2V_2C_2 \quad (12)$$

SOLUTION FOR THE STABLE STATE

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At steady - state:

$$a_{11}C_1 + a_{12}C_2 = W_1 \qquad (13)$$

$$a_{21}C_1 + a_{22}C_2 = W_2 \qquad (14)$$

Where

$$a_{11} = Q_{12} + k_1V_1 \qquad a_{21} = -Q_{12}$$

$$a_{12} = -Q_{21} \qquad a_{22} = Q_{21} + Q_{23} + k_2V_2$$

Solution

Lake 1 $$C_1 = \frac{1}{a_{11} - (a_{21}a_{12}/a_{22})}W_1 + \frac{1}{a_{21} - (a_{11}a_{22}/a_{12})}W_2 \qquad (15)$$

Lake 2 $$C_2 = \frac{1}{a_{12} - (a_{11}a_{22}/a_{21})}W_1 + \frac{1}{a_{22} - (a_{21}a_{12}/a_{11})}W_2 \qquad (16)$$

SOLUTION FOR THE STABLE STATE

➢ The solution method for the system of reactor

Considering the response impact system of 3 lakes, the equation of the mass balance of system of reactor is written as follows:

$$a_{11}C_1 + a_{12}C_2 + a_{13}C_3 = W_1 \qquad (17)$$

$$a_{21}C_1 + a_{22}C_2 + a_{23}C_3 = W_2 \qquad (18)$$

$$a_{31}C_1 + a_{32}C_2 + a_{33}C_3 = W_3 \qquad (19)$$

The equation system is rewritten as follows: $[A]\{C\} = \{W\}$ (20)

where

$$[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \qquad \{C\} = \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} \qquad \{W\} = \begin{Bmatrix} W_1 \\ W_2 \\ W_3 \end{Bmatrix}$$

SOLUTION FOR THE STABLE STATE

➢ The solution method for the system of reactor (cont)

The solution of this equation system is as follows: $\{C\} = [A]^{-1}\{W\}$ (21)

where $[A]^{-1}$ is an inverse matrix. [A]

Using the two-matrix method, the equation (20) can be deployed as follows:

$$C_1 = a_{11}^{(-1)} W_1 + a_{12}^{(-1)} W_2 + a_{13}^{(-1)} W_3 \qquad (22)$$

$$C_2 = a_{21}^{(-1)} W_1 + a_{22}^{(-1)} W_2 + a_{23}^{(-1)} W_3 \qquad (23)$$

$$C_3 = a_{31}^{(-1)} W_1 + a_{32}^{(-1)} W_2 + a_{33}^{(-1)} W_3 \qquad (24)$$

Where $a_{i,j}^{(-1)}$ is coefficient in row i, column j in inverse matrix.

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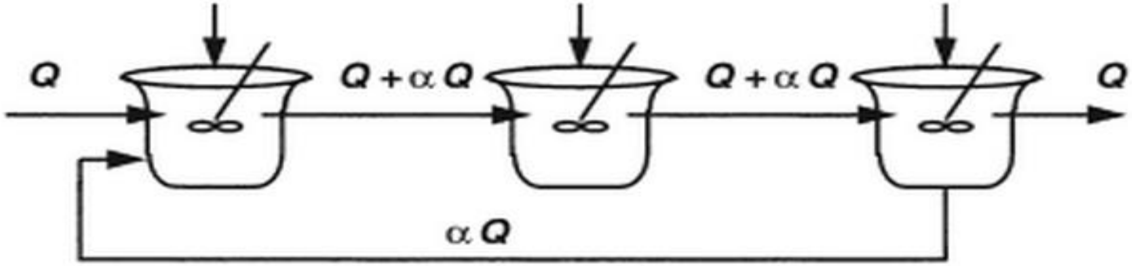
Example 2. Suppose that three lakes are connected in series



	Lake 1	Lake 2	Lake3
Volume, 10^6 m^3	2	4	3
Depth, m	3	7	3
Surface area, 10^6 m^2	0.667	0.571	1.000
Loading, kg/yr	2000	4000	1000

(a) If Q = 1×10^6 m^3/yr, $\alpha = 0.5$ and the rate of settles of pollutants is 10 m/yr. Calculate the concentration of each lake..

(b) Use an inverse matrix to determine the concentration of Lake 3 due to the load to Lake 2 contributing.

(c) Identify inverse matrix in case where $\alpha = 0$

Lời giải

(a) The steady-state mass balances for the three reactors can be written as:

$$0 = W_1 - (Q + \alpha Q)C_1 - vA_1C_1 + \alpha QC_3$$

$$0 = W_2 + (Q + \alpha Q)C_1 - (Q + \alpha Q)C_2 - vA_2C_2$$

$$0 = W_3 + (Q + \alpha Q)C_2 - (Q + \alpha Q)C_3 - vA_3C_3$$

Substituting the parameter values, the three simultaneous equations can be expressed in matrix form as

$$\begin{bmatrix} 8.17\times10^6 & 0 & -0.5\times10^6 \\ -1.5\times10^6 & 7.21\times10^6 & 0 \\ 0 & -1.5\times10^6 & 11.5\times10^6 \end{bmatrix} \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} = \begin{Bmatrix} 2\times10^9 \\ 4\times10^9 \\ 1\times10^9 \end{Bmatrix}$$

The inverse matrix is defined as follows

$$\begin{bmatrix} 1.23\times10^{-7} & 1.11\times10^{-9} & 5.33\times10^{-9} \\ 2.55\times10^{-8} & 1.39\times10^{-7} & 1.11\times10^{-9} \\ 3.33\times10^{-9} & 1.81\times10^{-8} & 8.71\times10^{-8} \end{bmatrix}$$

Which can be multiplied by (W) to give

$$\begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} = \begin{Bmatrix} 255 \\ 608 \\ 166 \end{Bmatrix}$$

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(b) The effect of lake 2 on the concentration of lake 3 is determined based on the coefficient $a_{32}^{(-1)}$.

$$a_{32}^{(-1)} = 1.81 \times 10^{-8} \, \mu g.L^{-1} / mg.yr^{-1}$$

The concentration of lake 3 due to the loading of lake 2 contributes:

$(1.81 \times 10^{-8}) \times (4 \times 10^{9}) = 72.5$ μg/L

(c) Where α = 0 , The equation system is written as a matrix as follows:

$$\begin{bmatrix} 7.67\times10^{6} & 0 & 0 \\ -1\times10^{6} & 6.71\times10^{6} & 0 \\ 0 & -1\times10^{6} & 11\times10^{6} \end{bmatrix} \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} = \begin{Bmatrix} 2\times10^{9} \\ 4\times10^{9} \\ 1\times10^{9} \end{Bmatrix}$$

The inverse matrix is defined as follows:

$$\begin{bmatrix} 1.30\times10^{-7} & 0 & 0 \\ 1.94\times10^{-8} & 1.49\times10^{-7} & 0 \\ 1.77\times10^{-9} & 1.35\times10^{-8} & 9.09\times10^{-8} \end{bmatrix}$$

SOLUTION FOR THE UNSTABLE STATE

Equations (11) and (12) in case W = 0 are written as follows:

Lake 1 $$\frac{dC_1}{dt} = -\alpha_{11}C_1 + \alpha_{12}C_2 \qquad (25)$$

Lake 2 $$\frac{dC_2}{dt} = \alpha_{21}C_1 - \alpha_{22}C_2 \qquad (26)$$

Where

$$\alpha_{11} = \frac{Q_{12}}{V_1} + k_1 \qquad \alpha_{12} = \frac{Q_{21}}{V_1} \qquad \alpha_{21} = \frac{Q_{12}}{V_2} \qquad \alpha_{22} = \frac{Q_{23} + Q_{21}}{V_2} + k_2$$

At t = 0: $C_1 = C_{10}$ và $C_2 = C_{20}$, then the general solution can be developed:

Lake 1 $$C_1 = C_{1f}e^{-\lambda_f t} + C_{1s}e^{-\lambda_s t} \qquad (27)$$

Lake 2 $$C_2 = C_{2f}e^{-\lambda_f t} + C_{2s}e^{-\lambda_s t} \qquad (28)$$

SOLUTION FOR THE UNSTABLE STATE

Where

λ are eigenvalue and is defined as follows.

$$\begin{matrix}\lambda_f \\ \lambda_s\end{matrix} = \frac{(\alpha_{11}+\alpha_{22}) \pm \sqrt{(\alpha_{11}+\alpha_{22})^2 - 4(\alpha_{11}\alpha_{22}-\alpha_{12}\alpha_{21})}}{2}$$

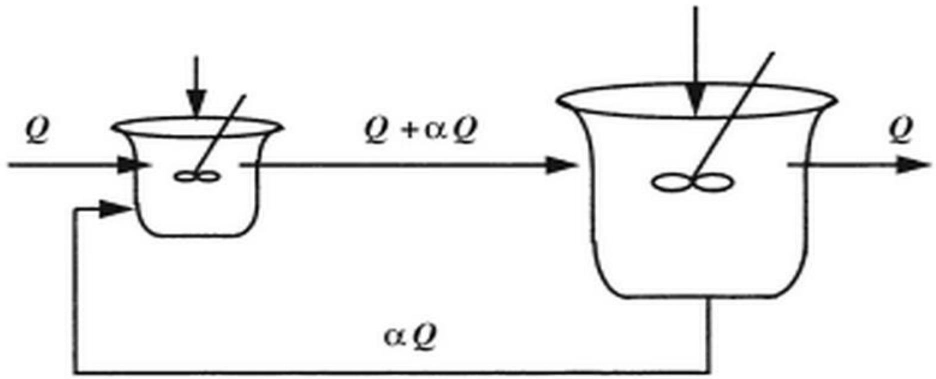
And the coefficients is

$$C_{1f} = \frac{(\lambda_f - \alpha_{22})C_{10} - \alpha_{12}C_{20}}{\lambda_f - \lambda_s} \qquad C_{1s} = \frac{\alpha_{12}C_{20} - (\lambda_s - \alpha_{22})C_{10}}{\lambda_f - \lambda_s}$$

$$C_{2f} = \frac{-\alpha_{21}C_{10} + (\lambda_f - \alpha_{11})C_{20}}{\lambda_f - \lambda_s} \qquad C_{2s} = \frac{-(\lambda_s - \alpha_{11})C_{20} + \alpha_{21}C_{10}}{\lambda_f - \lambda_s}$$

Based on the general solution, we realize that the resilience of the system depends on the magnitude of its own values. Note that $\lambda_f > \lambda_s$ và λ_f, λ_s Often used to refer to eigenvalues "fast" and "slow".

Example, 3. For a system of 2 lakes with the same characteristics as shown as below.



	Hồ 1	Hồ 2
Volume, 10^6 m^3	0.2	10
Depth, m	4	7
Surface area, 10^6 m^2	0.05	0.5
Load, kg/yr	2000	4000

(a) If $Q = 1 \times 10^6$ m^3/yr, $\alpha = 0.5$ and the rate of settles of pollutant is10 m/yr. Determined the concentration of each lake.

(b) Use the concentration value calculated in sentence (a) as the original value, determining the concentration movement over time of each lake.

Solution

(a) The solution is similar to example 2, the concentration in the steady- state of each lake:

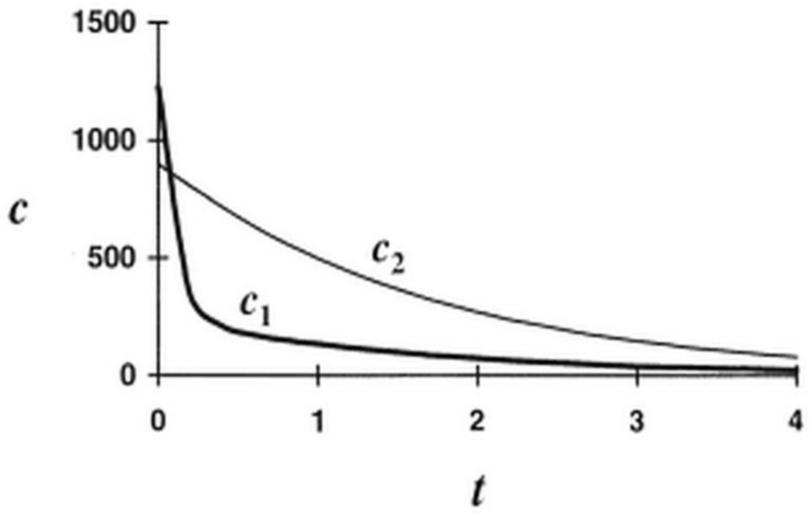
$$\{C\} = \begin{Bmatrix} 1224.5 \\ 898 \end{Bmatrix}$$

(b) The concentration of each lake over time is determined as follows

$$C_1 = 981.24e^{-10.04t} + 243.25e^{-0.61t}$$

$$C_2 = -15.67e^{-10.04t} + 913.63e^{-0.61t}$$

The chart shows the concentration of each lake as follows



Based on the graph, because of the large eigenvalue of Lake 1 at the beginning, the Lake 1 concentration rapidly decreased before slowly recovered