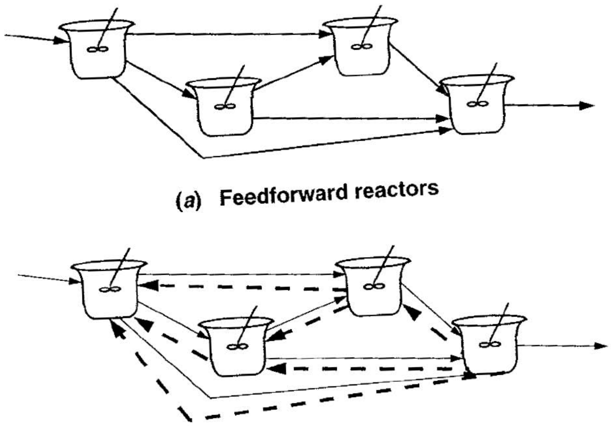
Lecture 5:
Feedforward Systems of Reactors

- To develop steady state and time variable solutions for several reactors
- To apply these solutions to a series of lakes

Reactors Connected in Series

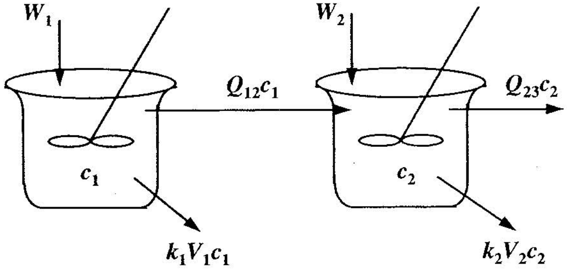


(a) Feedforward reactors

(b) Feedback reactors

- Feedforward reactor (w/o feedback)
- Feedback reactors

Lakes in Series

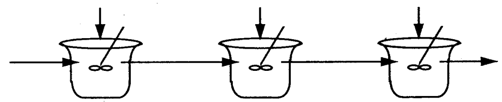


- Mass balances are:

$$V_1 (dc_1/dt) = W_1 - Q_{12}c_1 - k_1V_1c_1$$
$$V_2 (dc_2/dt) = W_2 + Q_{12}c_1 - Q_{23}c_2 - k_2V_2c_2$$

Example 3.1: Lakes in Series

EXAMPLE 5.1. LAKES IN SERIES. Suppose that three lakes connected in series have the following characteristics:



		1		2		3	
Volume, 10^6 m^3		2		4		3	
Mean depth, m		3		7		3	
Surface area, 10^6 m^2		0.667		0.571		1.000	
Loading, kg yr^{-1}		2000		4000		1000	
Flow, 10^6 m^3 yr^{-1}	1.0		1.0		1.0		1.0

If the pollutant settles at a rate of 10 m yr^{-1},

(*a*) Calculate the steady-state concentration in each of the reactors.

(*b*) Determine how much of the concentration in the third reactor is due to the loading to the second reactor.

Solution: (*a*) The concentration for the reactors can be determined by

$$c_1 = \frac{W_1}{Q_{12} + vA_1} = \frac{2 \times 10^9}{1.0 \times 10^6 + (10 \times 0.667 \times 10^6)} = 260.76\ \mu g\ L^{-1}$$

$$c_2 = \frac{W_2}{Q_{23} + vA_2} + \frac{Q_{12}c_1}{Q_{23} + vA_2}$$

$$= \frac{4 \times 10^9}{1.0 \times 10^6 + (10 \times 0.571 \times 10^6)} + \frac{1.0 \times 10^6(260.76)}{1.0 \times 10^6 + (10 \times 0.571 \times 10^6)}$$

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

$$c_3 = \frac{W_3}{Q_{34} + vA_3} + \frac{Q_{23}c_2}{Q_{34} + vA_3}$$

$$= \frac{1 \times 10^9}{1 \times 10^6 + (10 \times 1 \times 10^6)} + \frac{1.0 \times 10^6(634.99)}{1 \times 10^6 + (10 \times 1 \times 10^6)}$$

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

(*b*) The determination of how much of the third reactor's concentration is due to the loading to the second reactor can be established by inspecting the solution for c_2 above. As can be seen, 596.13 $\mu g\ L^{-1}$ of c_2 is due to direct loadings (that is, W_2), whereas 38.86 is due to the loadings to reactor 1. Therefore the effect of the second reactor on the third reactor can be calculated as

$$c_3(\text{due to loading to reactor 2}) = \frac{1.0 \times 10^6(596.13)}{1 \times 10^6 + (10 \times 1 \times 10^6)} = 54.19\ \mu g\ L^{-1}$$

Cascade Model

- Series of reactors which are identical in size and flow

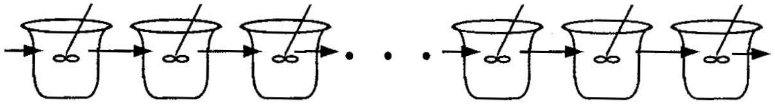
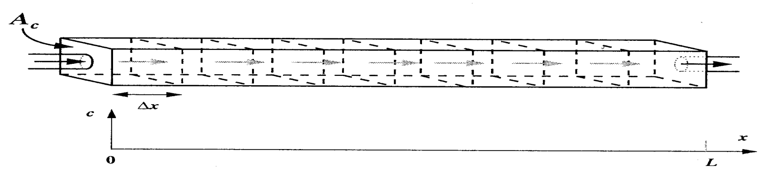


FIGURE 5.3
Cascade of CSTRs.

$$c_n = (Q/Q+kV)^n \times c_0$$

Example 3.2: Cascade Model in Elongated Tank

EXAMPLE 5.2. CASCADE MODEL OF AN ELONGATED TANK. Use the cascade model to simulate the steady-state distribution of concentration in an elongated tank.



The tank has cross-sectional area $A_c = 10\ \text{m}^2$, length $L = 100$ m, velocity $U = 100\ \text{m hr}^{-1}$, and first-order reaction rate $k = 2\ \text{hr}^{-1}$. The inflow concentration is $1\ \text{mg L}^{-1}$. Use $n = 1, 2, 4$, and 8 CSTRs to approximate the tank. Plot the results.

Solution: As in Eq. 5.12, the model for such a system is

$$c_n = \left(\frac{Q}{Q + kV}\right)^n c_0$$

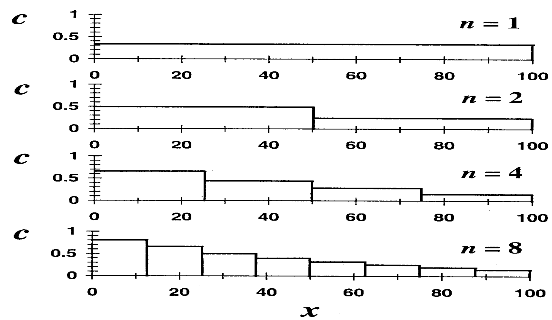


FIGURE 5.4
Approximation of an elongated tank by a series of n CSTRs.

Therefore for the single-segment approximation,

$$c(50) = \left[\frac{1000}{1000 + 2(1000)}\right] 1 = 0.3333\ \text{mg L}^{-1}$$

where $Q = UA = 100(10) = 1000$. Similarly for $n = 2$,

$$c(25) = \left[\frac{1000}{1000 + 2(500)}\right] 1 = 0.5\ \text{mg L}^{-1}$$

and

$$c(75) = \left[\frac{1000}{1000 + 2(500)}\right]^2 1 = 0.25\ \text{mg L}^{-1}$$

The other cases can be computed in similar fashion. The results, as summarized in Fig. 5.4, are interesting. As more (and smaller) reactors are used, the solution approaches a pattern that looks just like an exponential decay. We will explore this observation in more detail when we investigate models of elongated reactors in Lec. 9.

Time Variable

$$\frac{dc_1}{dt} = -\lambda_{11} c_1 \tag{5.13}$$

and

$$\frac{dc_2}{dt} = \lambda_{21} c_1 - \lambda_{22} c_2 \tag{5.14}$$

where

$$\lambda_{11} = \frac{Q_{12}}{V_1} + k_1 \tag{5.15}$$

$$\lambda_{21} = \frac{Q_{12}}{V_2} \tag{5.16}$$

$$\lambda_{22} = \frac{Q_{23}}{V_2} + k_2 \tag{5.17}$$

Again, as was the case for steady-state, the equations can be solved in sequence. If $c_1 = c_{10}$ and $c_2 = c_{20}$ at $t = 0$, the general solution for Eq. 5.13 can be developed as

$$c_1 = c_{10} e^{-\lambda_{11} t} \tag{5.18}$$

This result can be substituted into Eq. 5.14, which can then be solved for

$$c_2 = c_{20} e^{-\lambda_{22} t} + \frac{\lambda_{21} c_{10}}{\lambda_{22} - \lambda_{11}} \left(e^{-\lambda_{11} t} - e^{-\lambda_{22} t} \right) \tag{5.19}$$

Note also that this result is identical to the solution for a single lake with an exponential loading (Eq. 4.18).

Now suppose that there are a third and a fourth lake in series. For these cases solutions are (O'Connor and Mueller 1970, Di Toro 1972)

$$c_3 = c_{30} e^{-\lambda_{33} t} + \frac{\lambda_{32} c_{20}}{\lambda_{33} - \lambda_{22}} \left(e^{-\lambda_{22} t} - e^{-\lambda_{33} t} \right) + \frac{\lambda_{32} \lambda_{21} c_{10}}{\lambda_{22} - \lambda_{11}} \left(\frac{e^{-\lambda_{11} t} - e^{-\lambda_{33} t}}{\lambda_{33} - \lambda_{11}} - \frac{e^{-\lambda_{22} t} - e^{-\lambda_{33} t}}{\lambda_{33} - \lambda_{22}} \right) \tag{5.20}$$

and

$$\begin{aligned} c_4 = {} & c_{40} e^{-\lambda_{44} t} + \frac{\lambda_{43} c_{30}}{\lambda_{44} - \lambda_{33}} \left(e^{-\lambda_{33} t} - e^{-\lambda_{44} t} \right) \\ & + \frac{\lambda_{43} \lambda_{32} c_{20}}{\lambda_{33} - \lambda_{22}} \left(\frac{e^{-\lambda_{22} t} - e^{-\lambda_{44} t}}{\lambda_{44} - \lambda_{22}} - \frac{e^{-\lambda_{33} t} - e^{-\lambda_{44} t}}{\lambda_{44} - \lambda_{33}} \right) \\ & + \frac{\lambda_{43} \lambda_{32} \lambda_{21} c_{10}}{(\lambda_{22} - \lambda_{11})(\lambda_{33} - \lambda_{11})} \left(\frac{e^{-\lambda_{11} t} - e^{-\lambda_{44} t}}{\lambda_{44} - \lambda_{11}} - \frac{e^{-\lambda_{33} t} - e^{-\lambda_{44} t}}{\lambda_{44} - \lambda_{33}} \right) \\ & - \frac{\lambda_{43} \lambda_{32} \lambda_{21} c_{10}}{(\lambda_{22} - \lambda_{11})(\lambda_{33} - \lambda_{22})} \left(\frac{e^{-\lambda_{22} t} - e^{-\lambda_{44} t}}{\lambda_{44} - \lambda_{22}} - \frac{e^{-\lambda_{33} t} - e^{-\lambda_{44} t}}{\lambda_{44} - \lambda_{33}} \right) \end{aligned} \tag{5.21}$$

Time Variable (Cont.)

BOX 5.1. Efficient Schemes to Compute Concentrations for Serial Systems

Inspection of Eqs. 5.18 to 5.21 suggests a pattern that Di Toro (1972) expressed as a recurrence relation. For example for the case where only the first lake has an initial condition c_{10}, the equations can be reformulated as

$$c_1(t, \lambda_{11}) = c_{10}e^{-\lambda_{11}t} \tag{5.22}$$

$$c_2(t, \lambda_{11}, \lambda_{22}) = \frac{\lambda_{21}}{\lambda_{22} - \lambda_{11}}[c_1(t, \lambda_{11}) - c_1(t, \lambda_{22})] \tag{5.23}$$

$$c_3(t, \lambda_{11}, \lambda_{22}, \lambda_{33}) = \frac{\lambda_{32}}{\lambda_{33} - \lambda_{22}}[c_2(t, \lambda_{11}, \lambda_{22}) - c_2(t, \lambda_{11}, \lambda_{33})] \tag{5.24}$$

$$c_4(t, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{44}) = \frac{\lambda_{43}}{\lambda_{44} - \lambda_{33}}[c_3(t, \lambda_{11}, \lambda_{22}, \lambda_{33}) - c_3(t, \lambda_{11}, \lambda_{22}, \lambda_{44})] \tag{5.25}$$

The sequence can be generalized further for the case of the nth reactor,

$$c_n(t, \lambda_{11}, \ldots, \lambda_{n-1,n-1}, \lambda_{n,n}) = \prod_{j=1}^{n-1} \lambda_{j+1,j} \sum_{i=1}^{n} \frac{c_1(t, \lambda_{i,i})}{\prod_{j=1(j \neq i)}^{n} (\lambda_{j,j} - \lambda_{i,i})} \tag{5.26}$$

Di Toro (1972) further showed that this form requires 2^{n-1} evaluations of the c_1 function (Eq. 5.22). Since there are only n independent values of this function, Eq. 5.26 is inefficient. He then offered a more efficient version based on a partial-fraction expansion. The general form of this factored version is

$$c_n(t, \lambda_{11}, \ldots, \lambda_{n-1,n-1}, \lambda_{n,n}) = \prod_{j=1}^{n-1} \lambda_{j+1,j} \sum_{i=1}^{n} \frac{c_1(t, \lambda_{i,i})}{\prod_{j=1(j \neq i)}^{n} (\lambda_{j,j} - \lambda_{i,i})} \tag{5.27}$$

Example 5.3: Temporal Response of Lakes in Series

EXAMPLE 5.3. TEMPORAL RESPONSE OF LAKES IN SERIES. During the late 1950s and early 1960s, nuclear weapons testing introduced large quantities of radioactive substances into the atmosphere. As Fig. E5.3-1 shows, this resulted in a fallout flux of these substances to the surface of the earth.

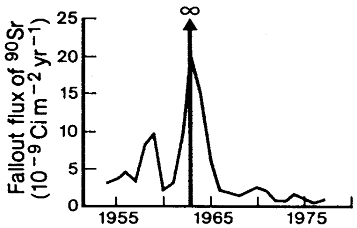


FIGURE E5.3-1
Fallout flux of ^{90}Sr to the Great Lakes (from Lerman 1972) along with the impulse load used to approximate the input.

Although the fallout has continued beyond the 1960s, the pronounced peak in 1963 allows idealization of the resulting load as an impulse function,

$$W(t) = J_{sr} A_s \delta(t - 1963)$$

where $J_{sr} = 70 \times 10^{-9}$ Ci m^{-2} (Ci denotes the radioactivity unit the curie)
A_s = lake surface area (m^2)
$\delta(t - 1963)$ = unit impulse function located at 1963

Predict the response of the Great Lakes to this flux if the half-life of ^{90}Sr is approximately 28.8 yr ($k = 0.0241$ yr^{-1}).

Solution: The Great Lakes can be represented as a series of reactors:

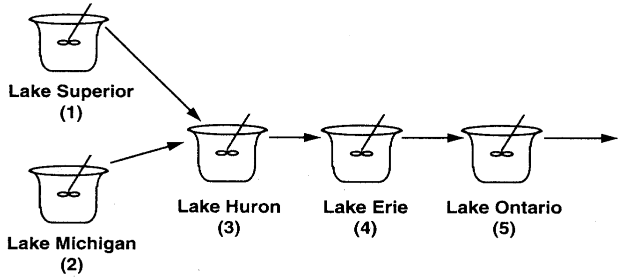


FIGURE E5.3-2

Example 5.3: Temporal Response of Lakes in Series

Both Lakes Superior and Michigan are "headwater" lakes. Their outflows feed into Lake Huron, which discharges to Lake Erie. Lake Ontario is the last lake in the chain. The parameters for the system are summarized as

Parameter	Units	Superior	Michigan	Huron	Erie	Ontario
Mean depth	m	146	85	59	19	86
Surface area	10^6 m^2	82,100	57,750	59,750	25,212	18,960
Volume	10^9 m^3	12,000	4,900	3,500	468	1,634
Outflow	10^9 m^3 yr^{-1}	67	36	161	182	212

The initial concentration in each lake in 1963 can be computed by

$$c_0 = \frac{J_{sr}}{H} \tag{E5.3.1}$$

where H = mean depth (m). The results are

	Units	Superior	Michigan	Huron	Erie	Ontario
c_0	10^{-9} Ci m^{-3}	0.479	0.824	1.186	3.684	0.814

Equations 5.18 through 5.21 can then be applied to compute the responses of each lake, and the total solution arrived at by summing the individual components. As in Eq. 5.18 the model for Lake Superior is

$$c_1 = 0.479e^{-0.02968t}$$

and for Lake Michigan is

$$c_2 = 0.824e^{-0.03145t}$$

Equation 5.18 is also used to predict how Lake Huron purges itself of its initial concentration. However, to compute the total response Eq. 5.19 is also employed to calculate the effect of Lakes Superior and Michigan on Huron's concentration:

$$c_3 = 1.186e^{-0.0701t} + \frac{0.01914(0.479)}{0.0701 - 0.02968}\left(e^{-0.02968t} - e^{-0.0701t}\right) + \frac{0.01029(0.824)}{0.0701 - 0.03145}\left(e^{-0.03145t} - e^{-0.0701t}\right)$$

The concentrations for the other lakes can be determined in a similar fashion. The results along with data are displayed in Fig. 5.5. The simulation duplicates the general trend of the data, with the exception that the computation decreases somewhat faster than the data. This is due, in part, to the use of an impulse forcing function to idealize the continuous loading function.

This analysis results in two conclusions:

- If two lakes receive an equal impulse flux of a pollutant, their response is inversely proportional to their depth (Eq. E5.3.1). This is the reason why shallow Lake Erie's initial concentration is about 4 times higher than for the other lakes.

Example 5.3: Temporal Response of Lakes in Series

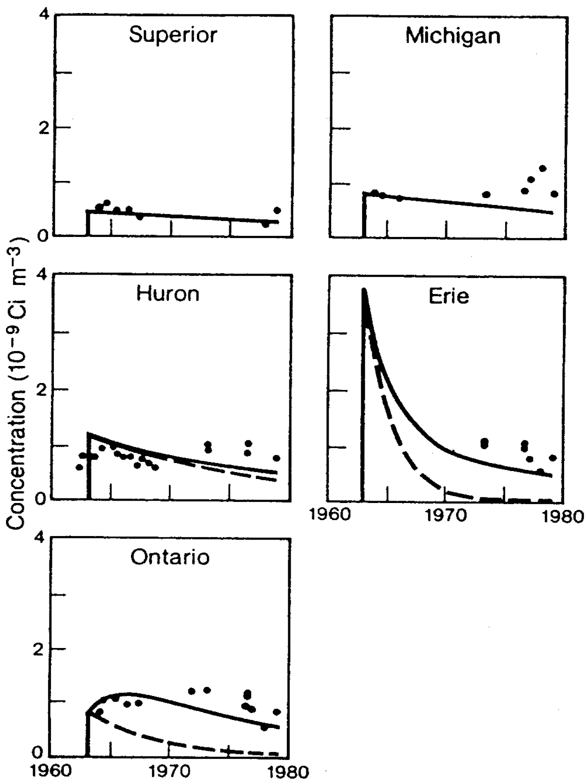
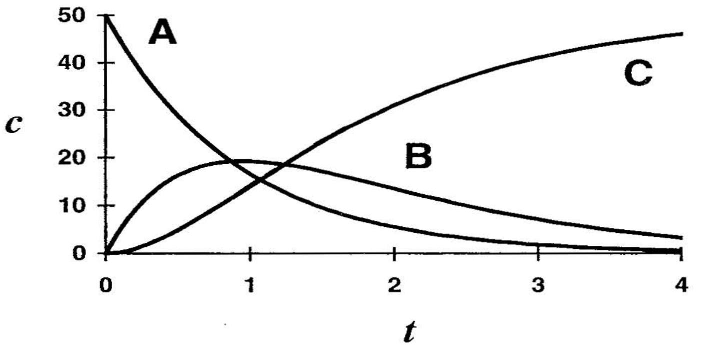


FIGURE 5.5
Response of the Great Lakes to an impulse loading of ^{90}Sr in 1963. Data (●) from Lerman (1972), Alberts and Wahlgren (1981), and International Joint Commission (1979). The dashed line represents the response of the lake to its own loading excluding the effect of upstream lakes.

- For a slowly decaying contaminant like ^{90}Sr, the upstream Great Lakes have a significant effect on the downstream lakes. The effect on Lake Ontario is so pronounced that its peak concentration does not occur in 1963 but lags 2 to 3 yr due to upstream effects.

Feedforward Reactions



$$\frac{dc_a}{dt} = -k_{ab}c_a \tag{5.30}$$

$$\frac{dc_b}{dt} = k_{ab}c_a - k_{bc}c_b \tag{5.31}$$

$$\frac{dc_c}{dt} = k_{bc}c_b \tag{5.32}$$

If $c_a = c_{a0}$, $c_b = c_c = 0$ at $t = 0$, the solution is

$$c_a = c_{a0}e^{-k_{ab}t} \tag{5.33}$$

$$c_b = \frac{k_{ab}c_{a0}}{k_{ab} - k_{bc}}\left(e^{-k_{bc}t} - e^{-k_{ab}t}\right) \tag{5.34}$$

$$c_c = c_{a0} - c_{a0}e^{-k_{ab}t} - \frac{k_{ab}c_{a0}}{k_{ab} - k_{bc}}\left(e^{-k_{bc}t} - e^{-k_{ab}t}\right) \tag{5.35}$$