第二單元:　水質模式的推導及利用

Session 2: Introduction to Water Quality Modeling

1. 質量守恆原理與環境模式
   Mass Balance Principle and Environmental Modeling Analysis

2. 水質模式分析相關的反應方程式及其係數
   Kinetics Formulation in Water Quality Modeling

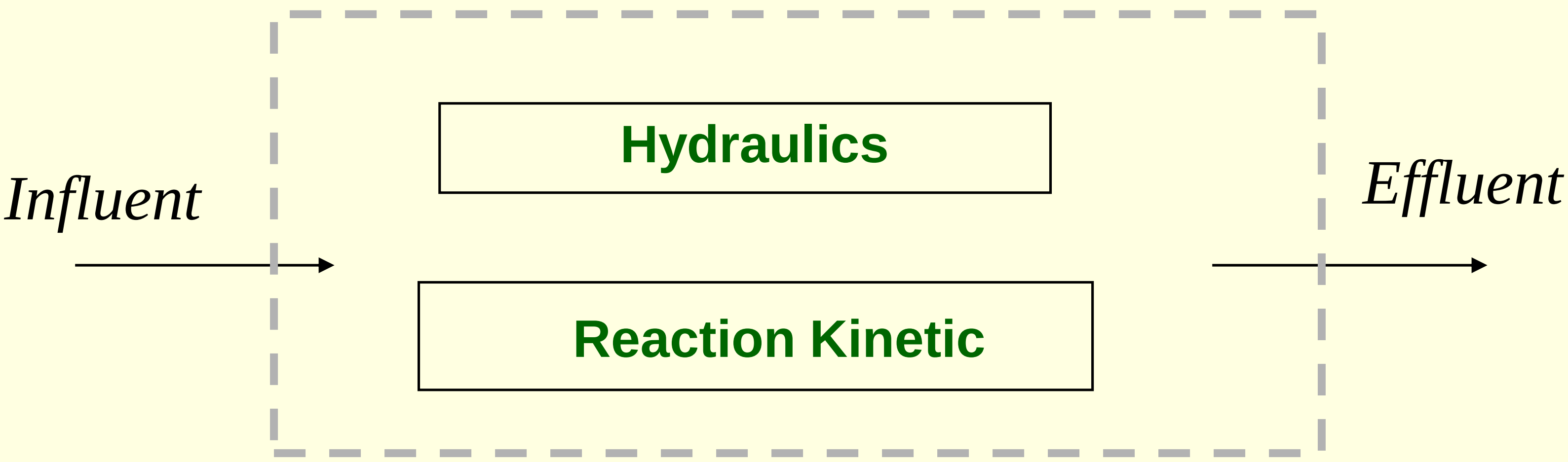
3. 理想反應器及簡易水質模式
   Simple Water Quality Models formulated as Ideal Reactors

4. 實例分析和小組討論
   Tutorial Session and Group Discussion

1.質量守恆原理與環境模式
Mass Balance Principle and Environmental Modeling Analysis

Environmental Modeling

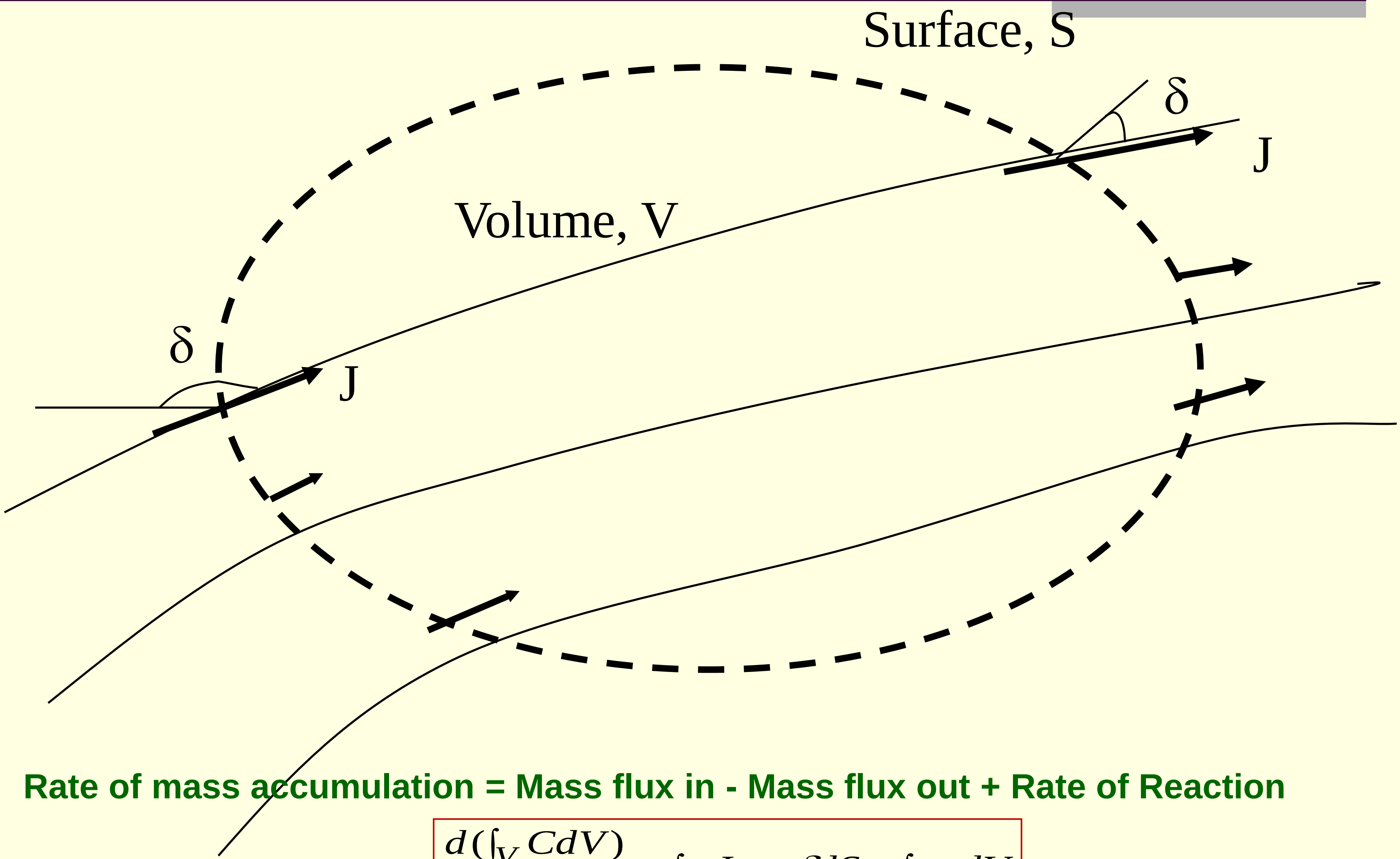
Environment Transport System



水質模式包含水體的水動力和各種自然反應，其推導是基於質量守恆原理.

An environmental model is formulated by combining the hydraulics and reaction kinetics on the basis of mass balance principle

質 量 守 恆 原 理及傳輸方程式
Mass Balance Principle and Transport Equation



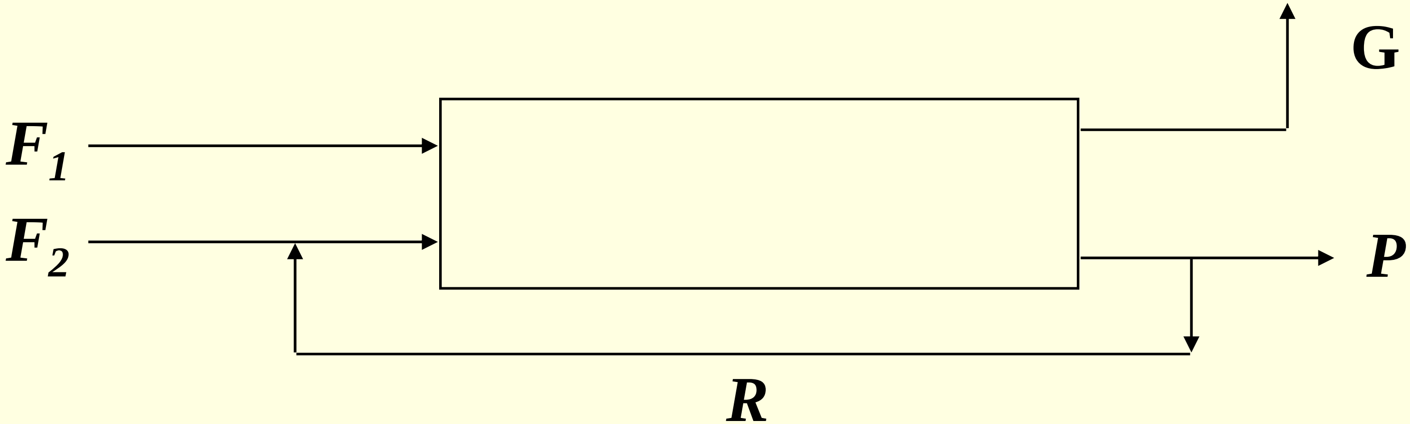
Rate of mass accumulation = Mass flux in - Mass flux out + Rate of Reaction

$$\frac{d(\int_V C dV)}{dt} = \int_S J \cos\delta \, dS + \int_V r dV$$

例題：應用質量守恆原理於穩定態問題

Example: Application of Mass Balance Principle to a Steady-state Transport problem

Consider the diagram and the data given below representing some sort of reaction between two liquids to produce a third liquid and a gas. The gas is produced at a mass ratio of 1 unit of gas for every 1000 units of liquid product.



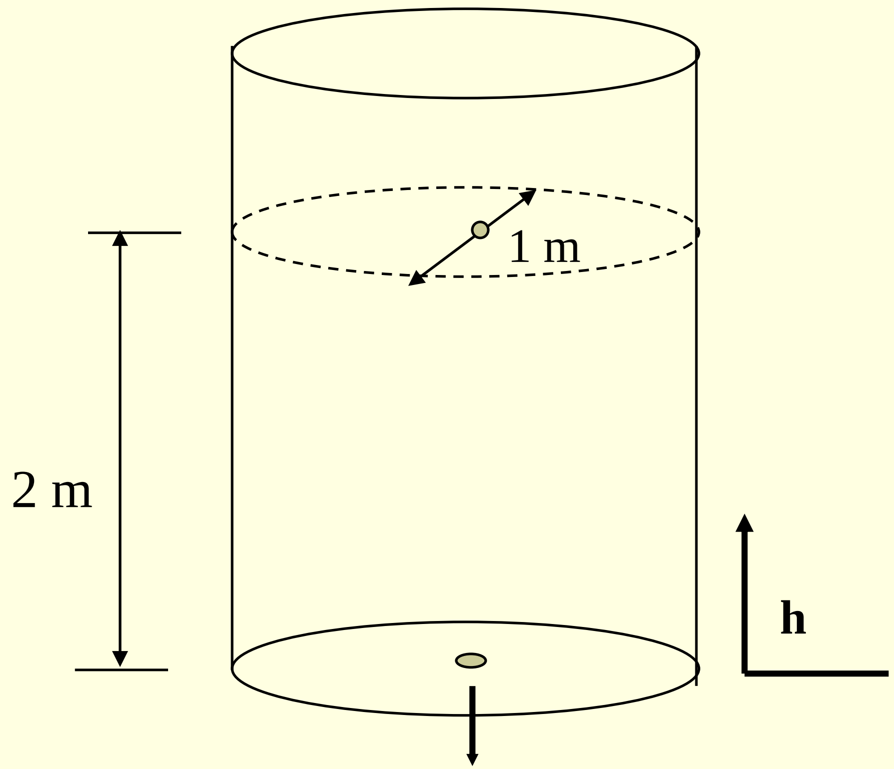
Stream	Flowrate	Density
Feed F_1	1000 L/min	1.5 kg/L
Feed F_2	5000 L/min	1.2 kg/L
Product P	Not given	1.3 kg/L
Recycle R	0.5 times P	same as P
Gas G	Not given	1.0 g/m^3

Calculate *P,G,* and *R* in L/min. What is the total flow rate into the reactor in kg/m?

例題：應用質量守恆原理於非穩定態問題 (1)排水問題

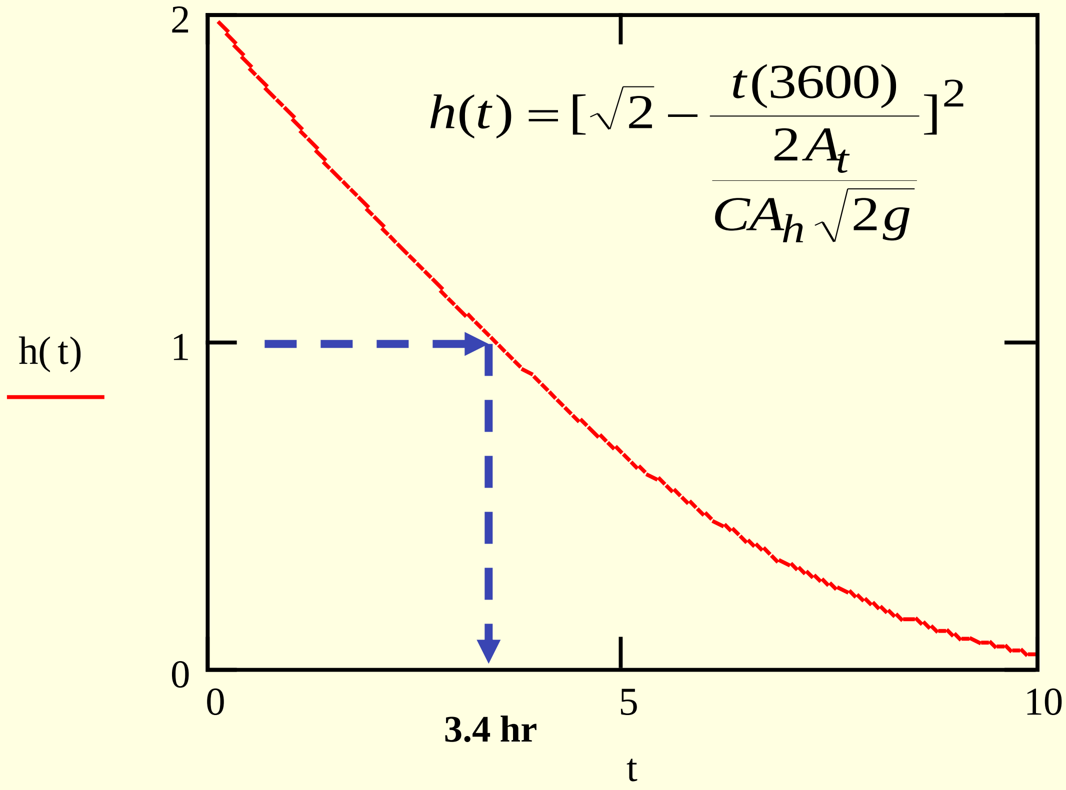
Example: Application of Mass Balance Principle to a Time-Variable Transport problem (1) Drainage Problem

A storage tank with a diameter of 1 m is filled to a depth of 2 m. If a 0.005-m-diameter hole were to develop in the bottom of the tank, The flow coefficient of the hole C = 0.61.



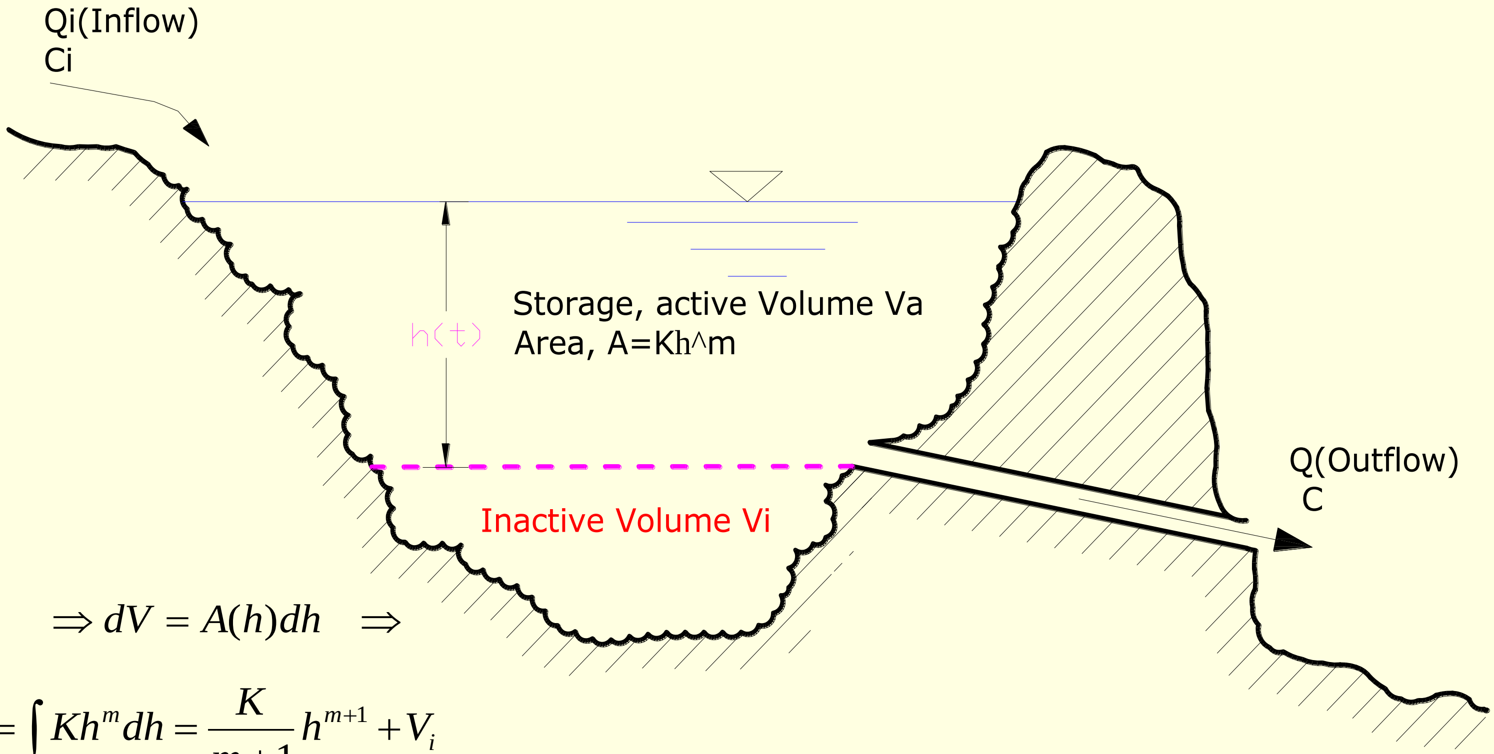
How long would it take for the liquid level to drop to 1.0 m?

Decline in water level as a function of time



例題：非穩定態問題（2)湖泊模式分析

Example: Time-Variable Problem (2) Lake Modeling



$$\frac{dV}{dt} = A(h)\frac{dh}{dt} \quad \Rightarrow dV = A(h)dh \quad \Rightarrow$$

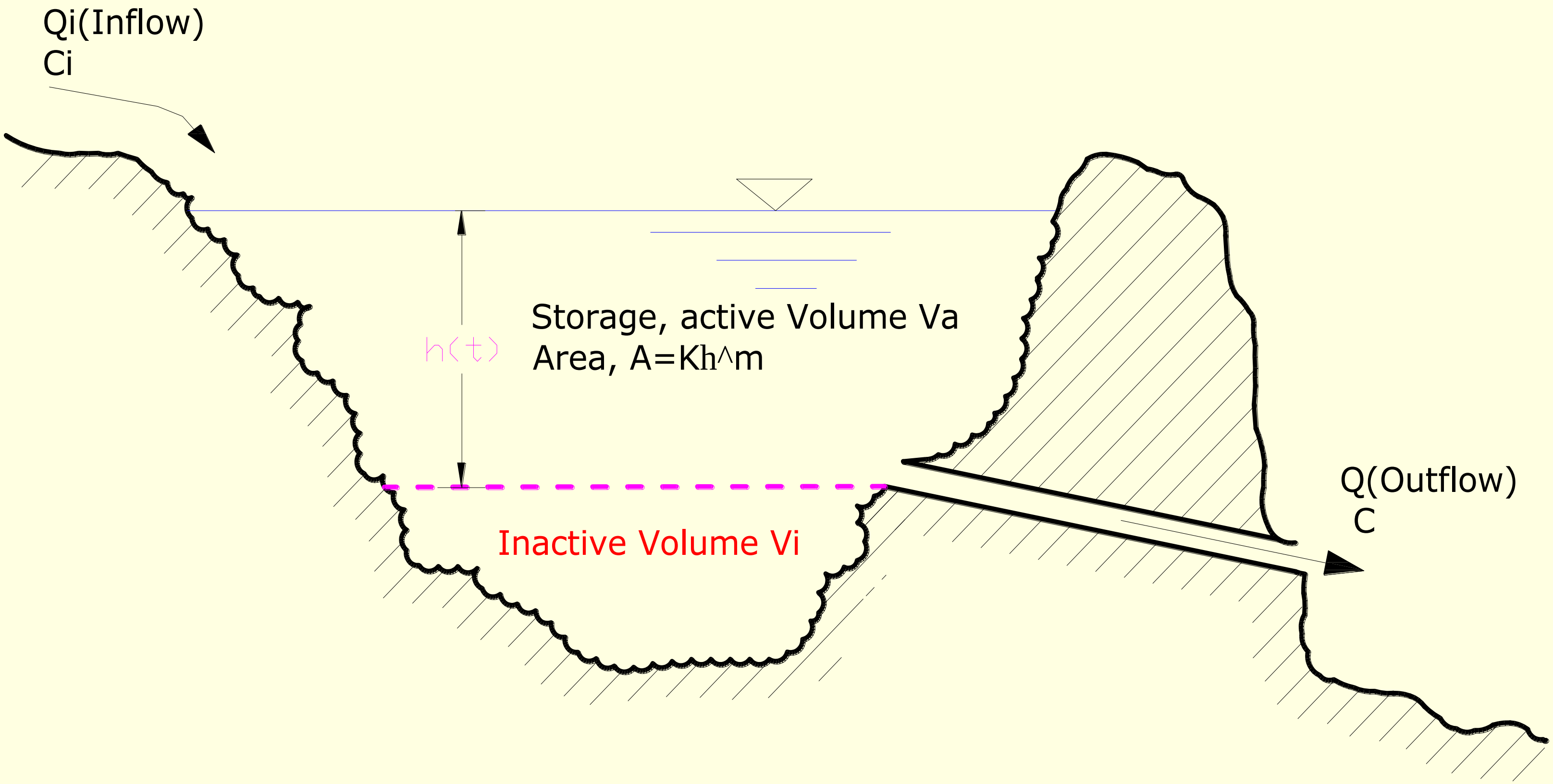
$$V = \int A(h)dh = \int Kh^m dh = \frac{K}{m+1}h^{m+1} + V_i$$

Here V_i is the inactive volume of detention pond,

we also can call it as dead volume.

$$\frac{dh}{dt} = \frac{Q_i - Q}{A(h)} = f(h,t)$$

水動力模式分析
Flow Modeling



質量守恆原理與水動力模式
Flow Routing

The mass balance analysis gives :

$$\frac{dV}{dt} = A(h)\frac{dh}{dt} = Q_i - Q \textbf{ Or, } \frac{dh}{dt} = \frac{Q_i - Q}{A(h)} = f(h,t)$$

dh/dt **can be approximated as**

$$\frac{dh}{dt} \approx \frac{h(t+\Delta t) - h(t)}{\Delta t}$$

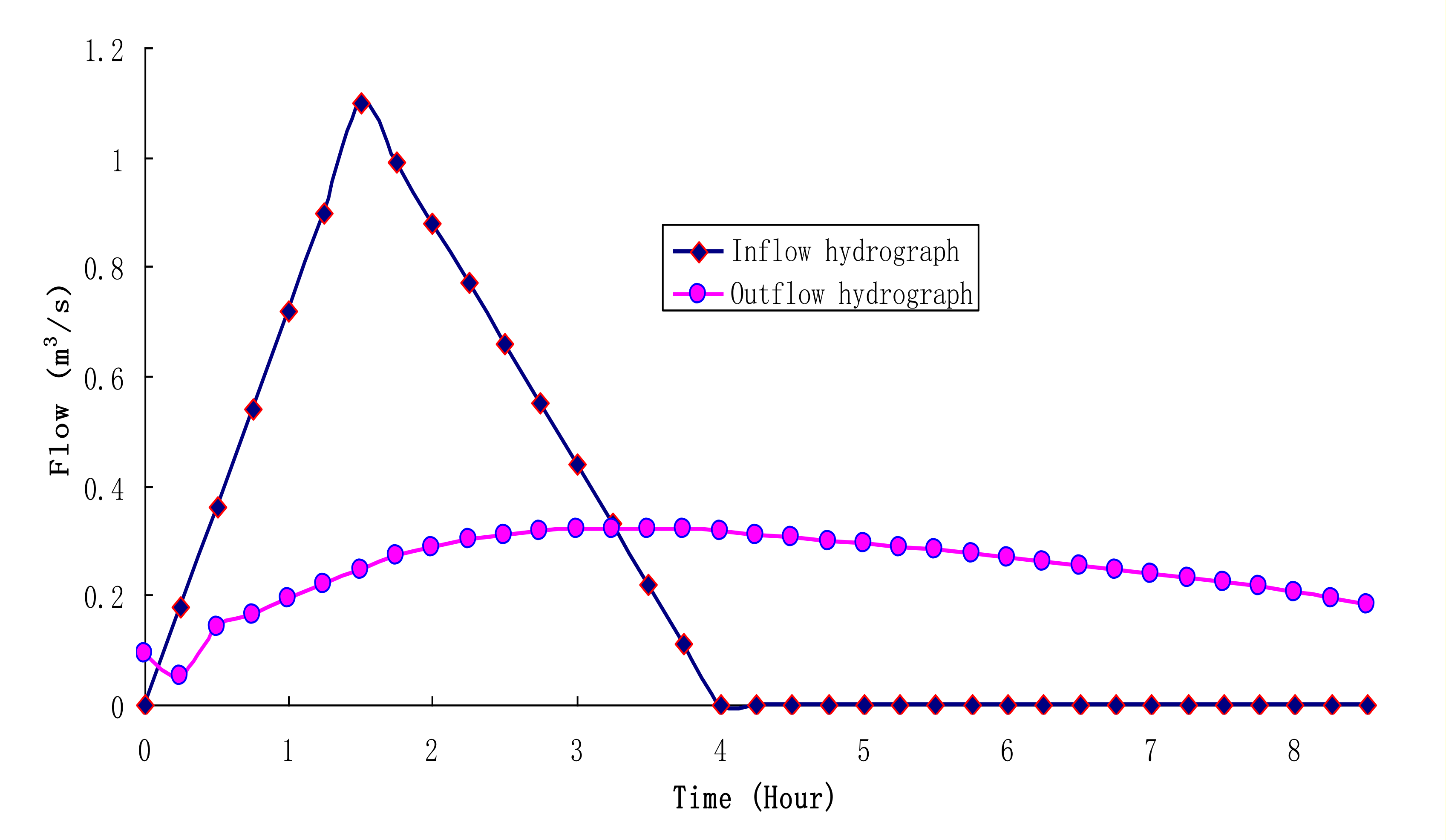
So, the depth at time (t + Δt) can be calculated with given depth at time t :

$$h(t+\Delta t) = h(t) + \frac{dh}{dt}\Delta t = h(t) + f(h,t)\Delta t$$

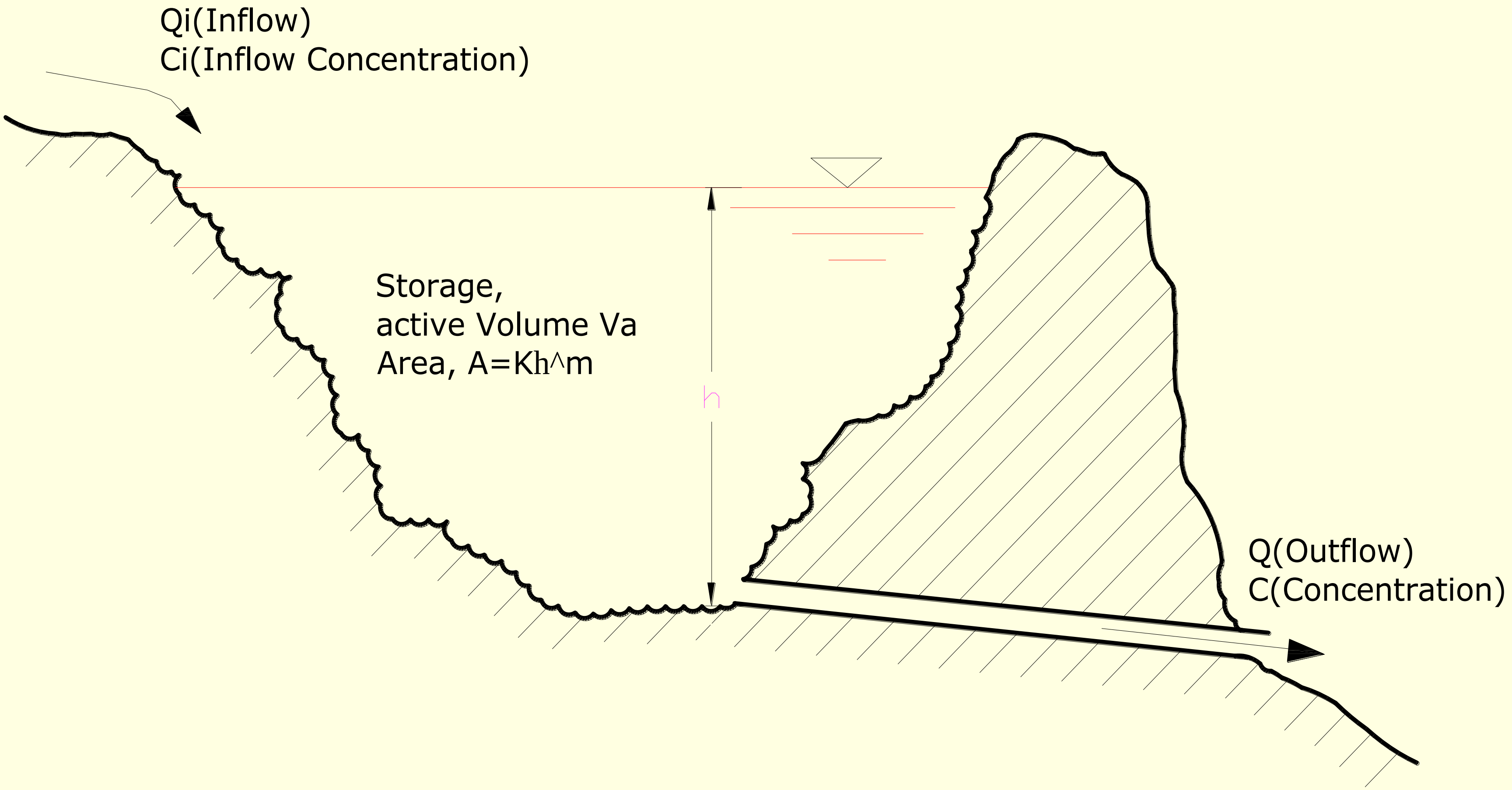
Flow Routing

Spreadsheet for Detention Pond Analysis						
(1)	(2)	(3)	(4)	(5)	(6)	(7)
Time	Q-In.	h(t)	Q-Out	A-Surf	dh/dt	h(t+dt)
(hr)	(m^3/s)	(m)	(m^3/s)	(m^2)	(m/s)	(m)
0	0	0.5000	0.0913	246.229	-0.0004	0.1661
0.25	0.18	0.1661	0.0527	113.852	0.0011	1.1728
0.5	0.36	1.1728	0.1399	447.216	0.0005	1.6157
0.75	0.54	1.6157	0.1642	559.654	0.0007	2.2201
1	0.72	2.2201	0.1925	699.061	0.0008	2.8992
1.25	0.9	2.8992	0.2200	842.665	0.0008	3.6255
1.5	1.1	3.6255	0.2460	985.413	0.0009	4.4055
1.75	0.99	4.4055	0.2712	1129.424	0.0006	4.9783
2	0.88	4.9783	0.2882	1230.322	0.0005	5.4112
2.25	0.77	5.4112	0.3005	1304.266	0.0004	5.7352
2.5	0.66	5.7352	0.3094	1358.448	0.0003	5.9675
2.75	0.55	5.9675	0.3156	1396.733	0.0002	6.1185
3	0.44	6.1185	0.3195	1421.389	0.0001	6.1948
3.25	0.33	6.1948	0.3215	1433.768	0.0000	6.2001
3.5	0.22	6.2001	0.3217	1434.629	-0.0001	6.1363
3.75	0.11	6.1363	0.3200	1424.282	-0.0001	6.0036
4	0	6.0036	0.3165	1402.650	-0.0002	5.8005
4.25	0	5.8005	0.3111	1369.263	-0.0002	5.5960
4.5	0	5.5960	0.3056	1335.289	-0.0002	5.3900
4.75	0	5.3900	0.2999	1300.691	-0.0002	5.1825
5	0	5.1825	0.2941	1265.430	-0.0002	4.9733
5.25	0	4.9733	0.2881	1229.459	-0.0002	4.7624
5.5	0	4.7624	0.2819	1192.728	-0.0002	4.5497
5.75	0	4.5497	0.2756	1155.179	-0.0002	4.3350
6	0	4.3350	0.2690	1116.747	-0.0002	4.1183
6.25	0	4.1183	0.2622	1077.358	-0.0002	3.8993
6.5	0	3.8993	0.2551	1036.926	-0.0002	3.6779
6.75	0	3.6779	0.2477	995.350	-0.0002	3.4538
7	0	3.4538	0.2401	952.514	-0.0003	3.2270
7.25	0	3.2270	0.2321	908.277	-0.0003	2.9970
7.5	0	2.9970	0.2236	862.471	-0.0003	2.7637
7.75	0	2.7637	0.2148	814.890	-0.0003	2.5265
8	0	2.5265	0.2053	765.279	-0.0003	2.2850
8.25	0	2.2850	0.1953	713.309	-0.0003	2.0386
8.5	0	2.0386	0.1845	658.554	-0.0003	1.7865

Inflow and Outflow Hydrographs



污染物傳輸模式分析
Transport Modeling

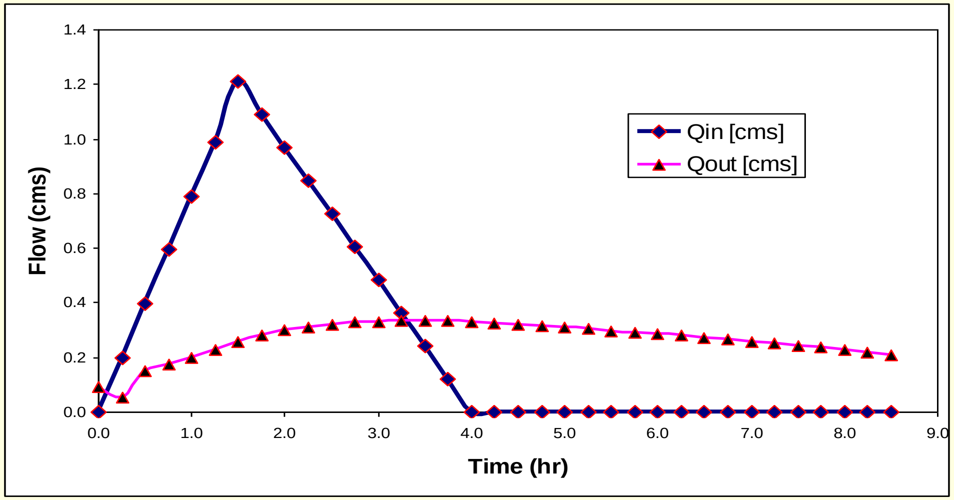


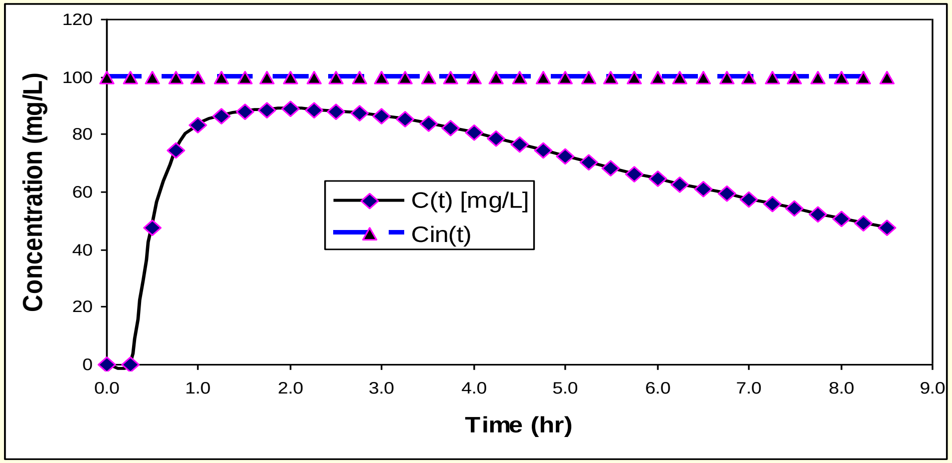
Transport Modeling

Spreadsheet for an Inflow/Outflow Water Quality Analysis of a Detention Pond

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
Time	**Qin**	***h(t)***	**Qout**	***A-surf***	***dh/dt***	***h(t + dt)***	**k**	**Cin**	**Flux-I**	**M(t)**	**C(t)**	**Flux-o**	**dM/dt**	**M(t+Δt)**
(hr)	**(m^3/s)**	**(m)**	**(m^3/s)**	**m^2**	**m/s**	**(m)**	**hr^{-1}**	**g/m^3**	**kg/hr**	**g**	**g/m^3**	**kg/hr**	**g/hr**	**g**
0	0	0.500	0.091	246.23	-0.0004	0.166	0.1	100	0	0	**0**	0	0	0
0.25	0.18	0.166	0.053	113.85	0.0011	1.173	0.1	100	64.8	0	**0**	0	64800	16200
0.5	0.36	1.173	0.140	447.22	0.0005	1.616	0.1	100	129.6	16200	**52.51**	26.45	101535	41583.65
0.75	0.54	1.616	0.164	559.65	0.0007	2.220	0.1	100	194.4	41584	**78.18**	46.21	144027	77590.32
1	0.72	2.220	0.192	699.06	0.0008	2.899	0.1	100	259.2	77590	**84.99**	58.89	192546	125726.9
1.25	0.9	2.899	0.220	842.67	0.0008	3.626	0.1	100	324	125727	**87.49**	69.28	242149	186264.1
1.5	1.1	3.626	0.246	985.41	0.0009	4.406	0.1	100	396	186264	**88.63**	78.49	298888	260986.1
1.75	0.99	4.406	0.271	1129.42	0.0006	4.978	0.1	100	356.4	260986	**89.17**	87.04	243260	321801
2	0.88	4.978	0.288	1230.32	0.0005	5.411	0.1	100	316.8	321801	**89.32**	92.68	191939	369785.7
2.25	0.77	5.411	0.301	1304.27	0.0004	5.735	0.1	100	277.2	369786	**89.07**	96.36	143860	405750.8
2.5	0.66	5.735	0.309	1358.45	0.0003	5.967	0.1	100	237.6	405751	**88.54**	98.61	98418	430355.3
2.75	0.55	5.967	0.316	1396.73	0.0002	6.119	0.1	100	198	430355	**87.78**	99.72	55244	444166.4
3	0.44	6.119	0.320	1421.39	0.0001	6.195	0.1	100	158.4	444166	**86.82**	99.88	14104	447692.5
3.25	0.33	6.195	0.322	1433.77	0.0000	6.200	0.1	100	118.8	447692	**85.69**	99.19	-25156	441403.6
3.5	0.22	6.200	0.322	1434.63	-0.0001	6.136	0.1	100	79.2	441404	**84.36**	97.69	-62633	425745.4
3.75	0.11	6.136	0.320	1424.28	-0.0001	6.004	0.1	100	39.6	425745	**82.81**	95.4	-98378	401150.8
4	0	6.004	0.317	1402.65	-0.0002	5.801	0.1	100	0	401151	**80.98**	92.28	-132397	368051.6
4.25	0	5.801	0.311	1369.26	-0.0002	5.596	0.1	100	0	368052	**78.78**	88.24	-125043	336790.9
4.5	0	5.596	0.306	1335.29	-0.0002	5.390	0.1	100	0	336791	**76.62**	84.3	-117976	307297
4.75	0	5.390	0.300	1300.69	-0.0002	5.183	0.1	100	0	307297	**74.51**	80.45	-111185	279500.8
5	0	5.183	0.294	1265.43	-0.0002	4.973	0.1	100	0	279501	**72.45**	76.71	-104658	253336.3
5.25	0	4.973	0.288	1229.46	-0.0002	4.762	0.1	100	0	253336	**70.43**	73.05	-98384	228740.3
5.5	0	4.762	0.282	1192.73	-0.0002	4.550	0.1	100	0	228740	**68.46**	69.48	-92353	205652.1
5.75	0	4.550	0.276	1155.18	-0.0002	4.335	0.1	100	0	205652	**66.52**	65.99	-86552	184014.1
6	0	4.335	0.269	1116.75	-0.0002	4.118	0.1	100	0	184014	**64.62**	62.57	-80971	163771.3
6.25	0	4.118	0.262	1077.36	-0.0002	3.899	0.1	100	0	163771	**62.75**	59.22	-75599	144871.5
6.5	0	3.899	0.255	1036.93	-0.0002	3.678	0.1	100	0	144871	**60.91**	55.94	-70425	127265.1
6.75	0	3.678	0.248	995.35	-0.0002	3.454	0.1	100	0	127265	**59.1**	52.71	-65438	110905.8
7	0	3.454	0.240	952.51	-0.0003	3.227	0.1	100	0	110906	**57.31**	49.53	-60624	95749.81
7.25	0	3.227	0.232	908.28	-0.0003	2.997	0.1	100	0	95750	**55.54**	46.4	-55972	81756.92
7.5	0	2.997	0.224	862.47	-0.0003	2.764	0.1	100	0	81757	**53.77**	43.29	-51467	68890.22
7.75	0	2.764	0.215	814.89	-0.0003	2.526	0.1	100	0	68890	**52**	40.21	-47094	57116.69
8	0	2.526	0.205	765.28	-0.0003	2.285	0.1	100	0	57117	**50.22**	37.12	-42835	46407.85
8.25	0	2.285	0.195	713.31	-0.0003	2.039	0.1	100	0	46408	**48.4**	34.03	-38669	36740.65
8.5	0	2.039	0.184	658.55	-0.0003	1.787	0.1	100	0	36741	**46.52**	30.89	-34567	28098.98

Inflow and Outflow Pollutograph and Pollutant Loading Curve





2.水質模式分析相關的反應方程式及其係數

Kinetics Formulation in Water Quality Modeling

Reaction Kinetics

A. Reaction Rate

$$r = \frac{dC}{dt} = kC^a$$

where

r = reaction rate

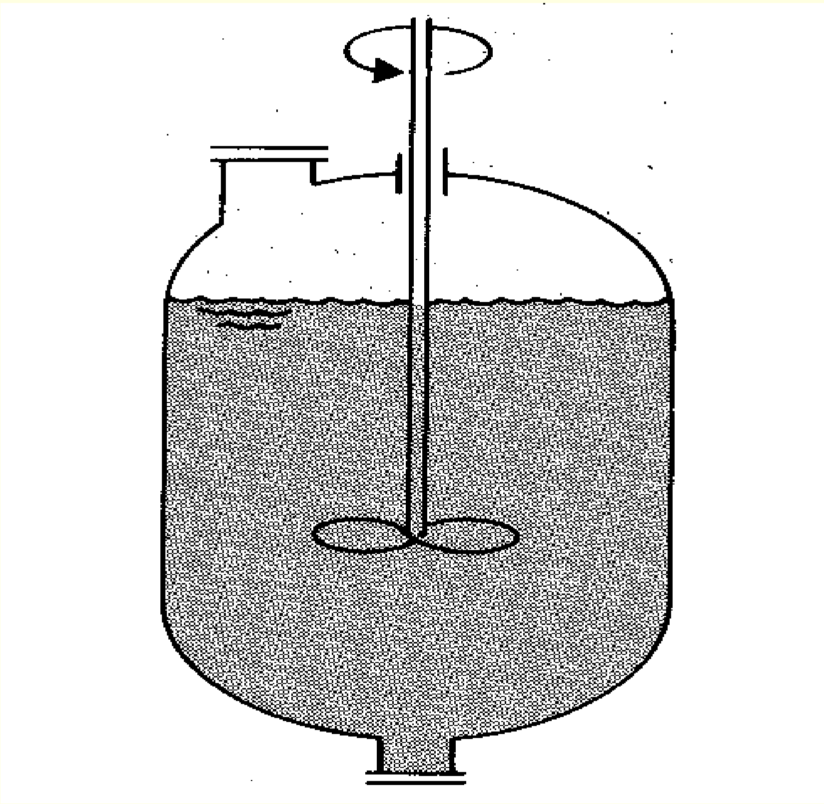
C = Concentration

k = Reaction rate constant

a = Empirical exponents (order of the reaction)

B. 反 應 方 程 推 導 過 程 中 的 Batch 實 驗

Batch Experiment and the Evaluation of Reaction Kinetics

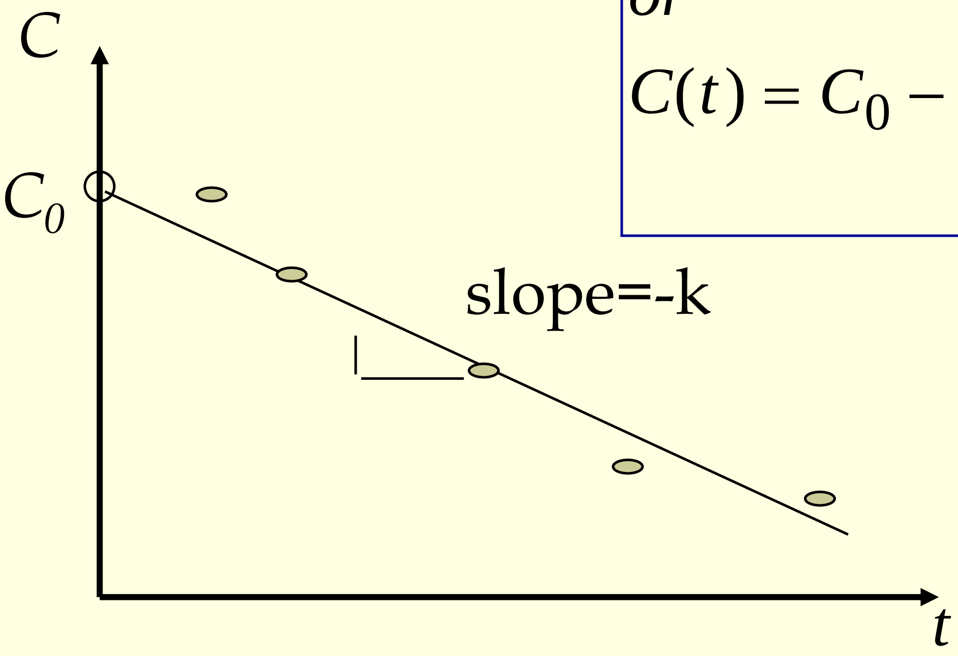


零 階 反 應 **Zero-order Reaction**

$$\frac{dC}{dt} = -kC^0 = -k$$

or

$$C(t) = C_0 - kt$$



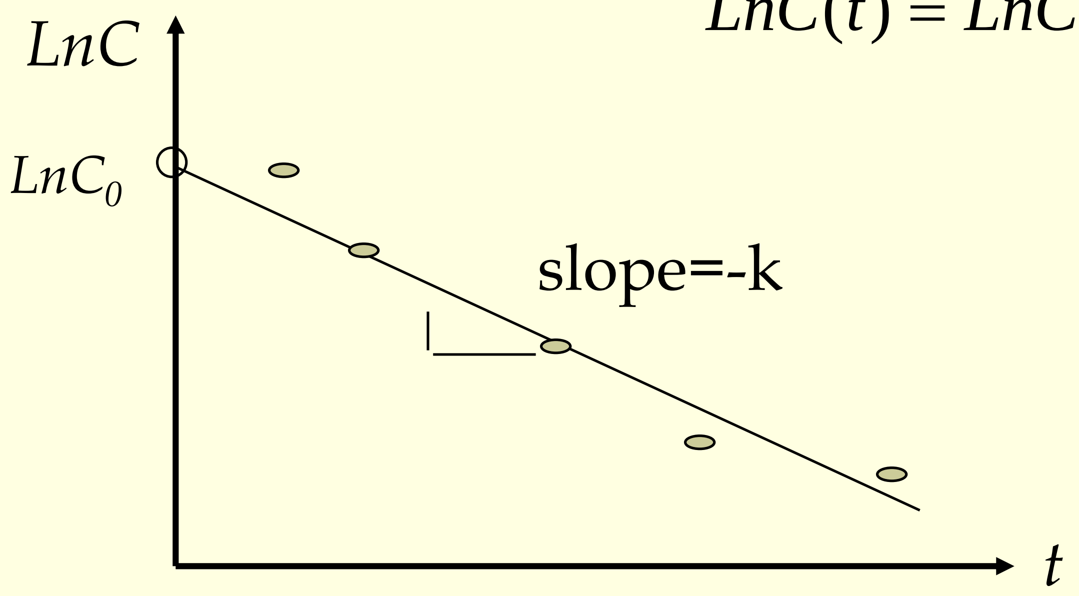
一階 反 應 **Zero-order Reaction**

$$\frac{dC}{dt} = -kC^1 = -kC$$

$$C(t) = C_0 \exp(-kt)$$

or

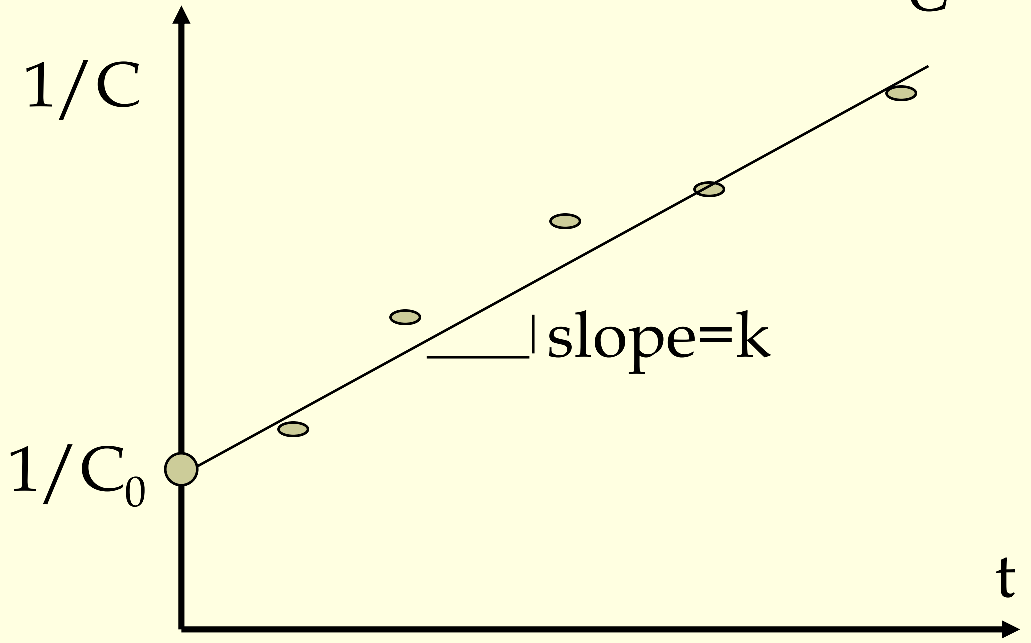
$$LnC(t) = LnC_o - kt$$



二階反應 **Second-order Reaction**

$$\frac{dC}{dt} = -kC^2$$

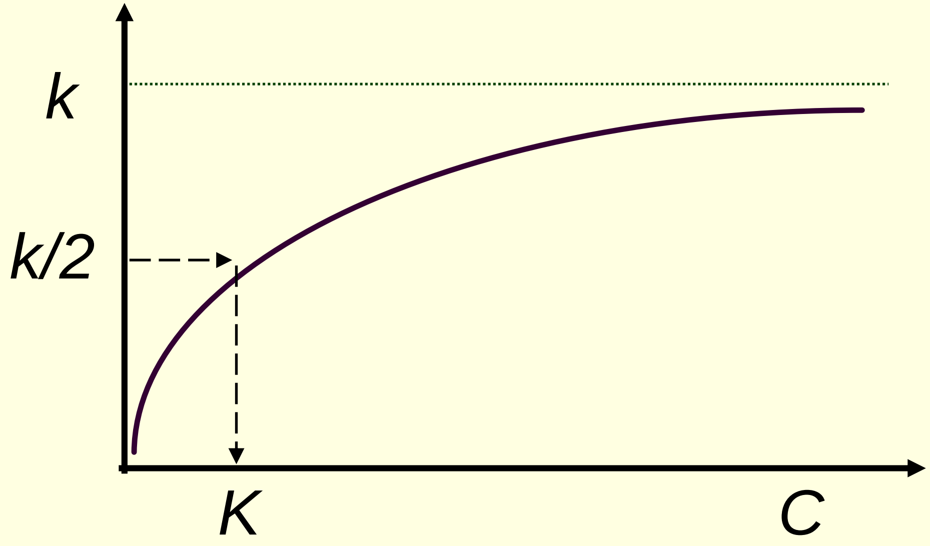
$$\frac{1}{C} = \frac{1}{C_0} + kt$$



飽和型反應 Saturation-type Kinetics

$$r = \frac{kC}{K + C}$$

k = *Max reaction rate constant*
K = *half-saturation constant*
C = *Pollutant concentration*



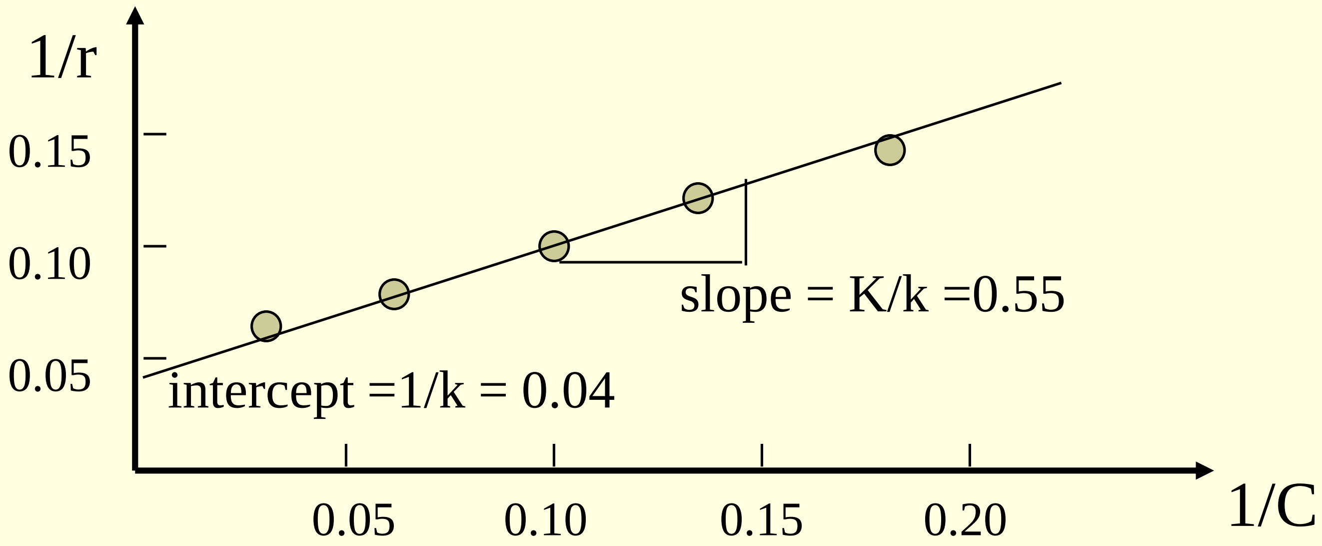
例題：利用實驗數據估求飽和型反應的數據值

Example: Determine rate constants of a saturation-type reaction

A bacterial growth experiment conducted at 20 ^{0}C in a batch reactor produced the following results:

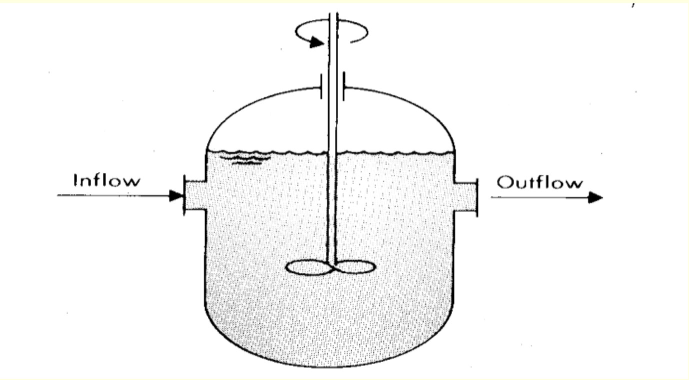
r (mg/L day)	16	12	10	8	7
C(mg/L)	30	15	10	7	6

Determine the maximum specific growth rate k and the half-saturation constant K.

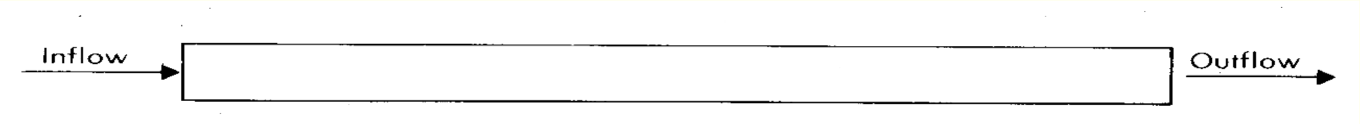


3.理想反應器及簡易水質模式的推導

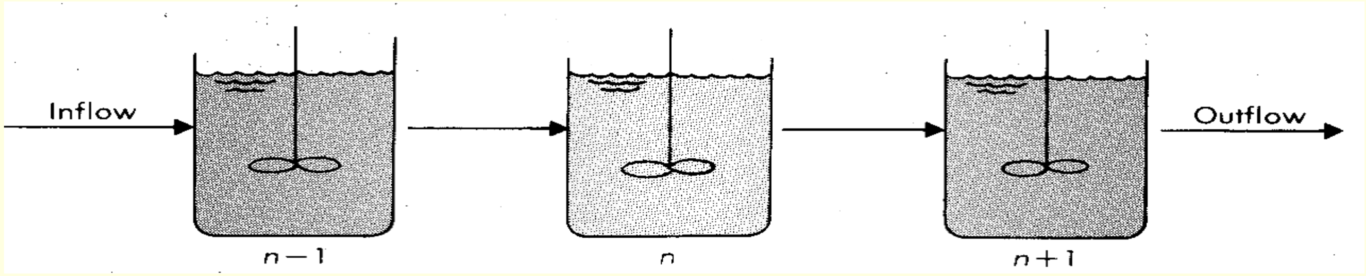
Simple Water Quality Models formulated as Ideal Reactors



(a) Complete-mix Reactor



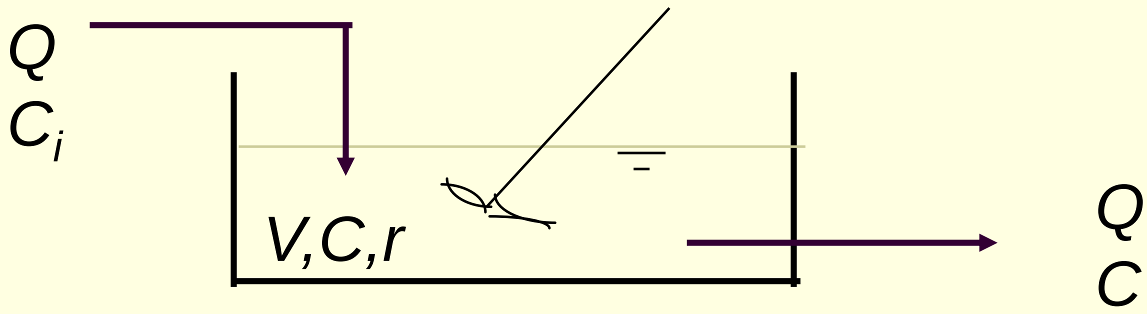
(b) Plug-flow Reactor



(c) Cascade of complete-mix Reactor

A. 完全混合反應器

Complete Stirred Tank Reactor (CSTR)



Mass Balance Principle:

Rate of Accumulation = Mass Flux In - Mass Flux Out + Reaction Rate

$$V\frac{dC}{dt} = QC_i - QC + Vr$$

For a first-order reaction, $r = -kC$ then,

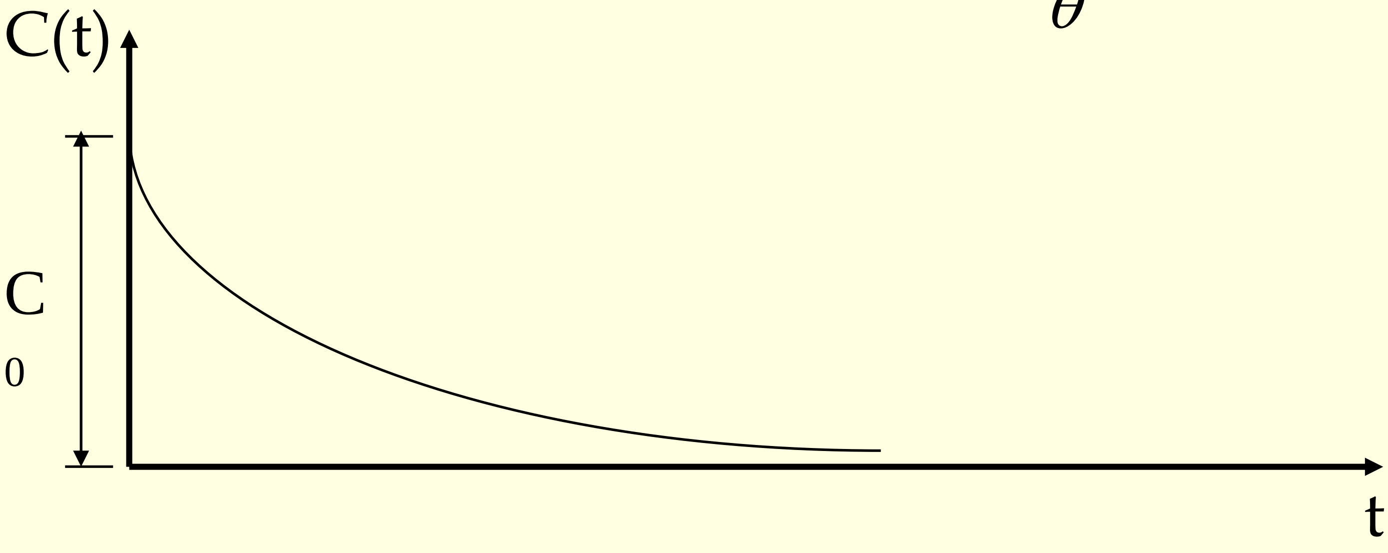
$$V\left(\frac{dC}{dt}\right) = QC_i - QC + V(-kC)$$

完全混合反應器模式接受一初始濃度的解析解

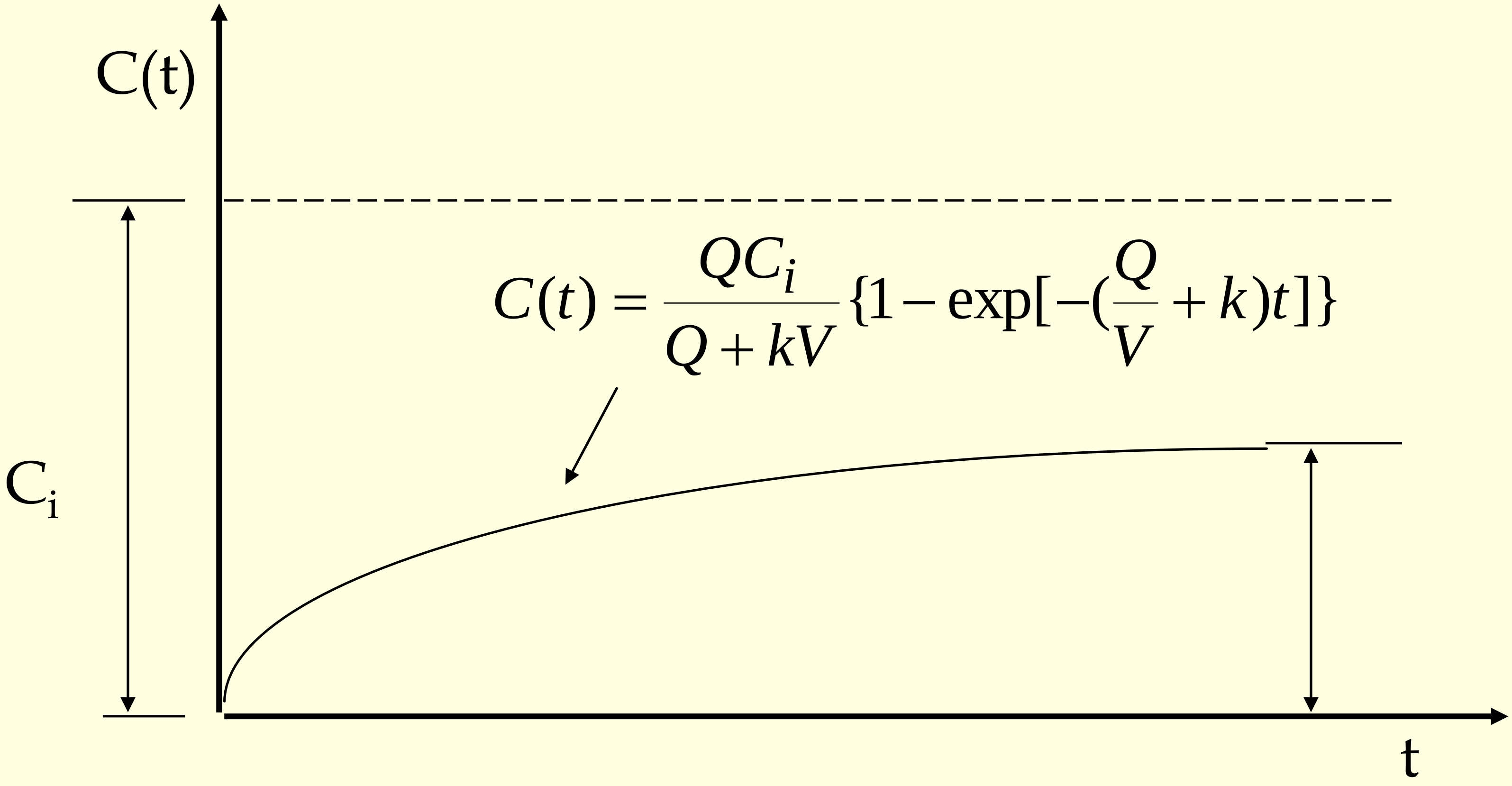
Solution of a CSTR Model with a Pulse Input

$$C(t) = C_0 \exp[-(\frac{Q}{V} + k)t]$$

$$or, C(t) = C_0 \exp[-(\frac{1}{\theta} + k)t]$$



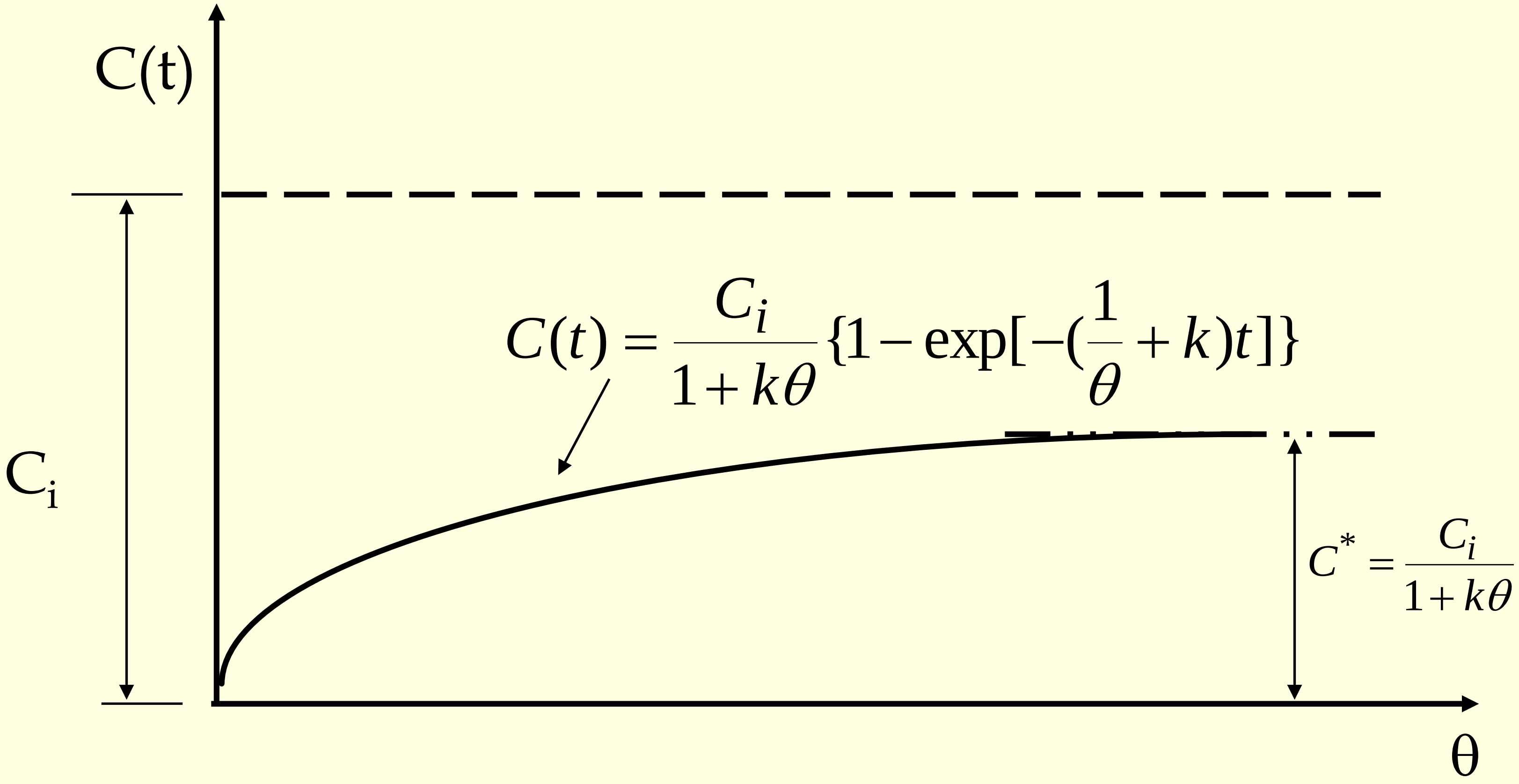
完全混合模式接受固定入流濃度的解析解
Solution of a CSTR Model with a constant continuous input



$$C(t) = \frac{QC_i}{Q + kV}\{1 - \exp[-(\frac{Q}{V} + k)t]\}$$

混合反應器平均停留時間 (θ＝ V/Q)

Solution expressed by mean residence time



C^* = Steady-state solution

線型理論與解析解的疊加
Linear System and the Principle of Superposition

Solution with a continuous input, *C_i*：

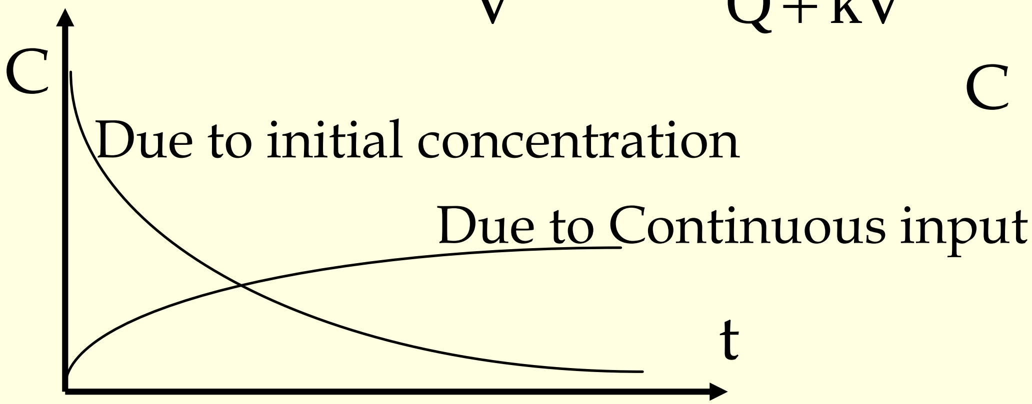
$$C(t) = \frac{QC_i}{Q + kV}\{1 - \exp[-(\frac{Q}{V} + k)t]\}$$

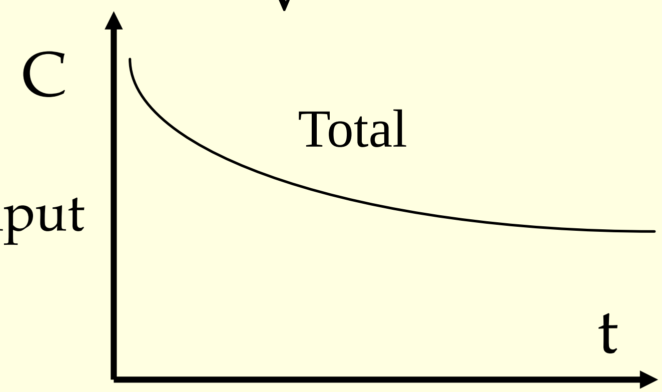
Solution with a pulse input or an initial concentration *C_0*:

$$C(t) = C_0 \exp[-(\frac{Q}{V}) + k)t]$$

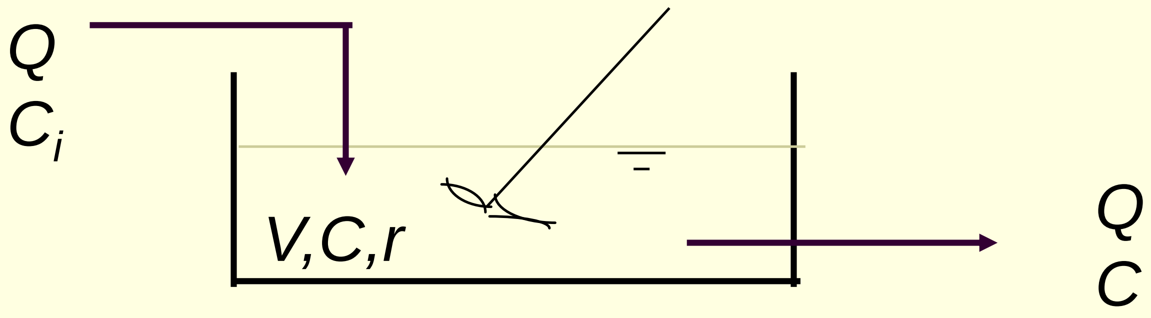
General solution to a completely mixed Reactor system:

$$C(t) = C_0 \exp[-(\frac{Q}{V} + k)t] + \frac{QC_i}{Q + kV}\{1 - \exp[-(\frac{Q}{V} + k)t]\}$$





完全混合反應器的線型系統分析
CSTR Linear Systems Modeling



$$V\left(\frac{dC}{dt}\right) = QC_i - QC + V(-kC)$$

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

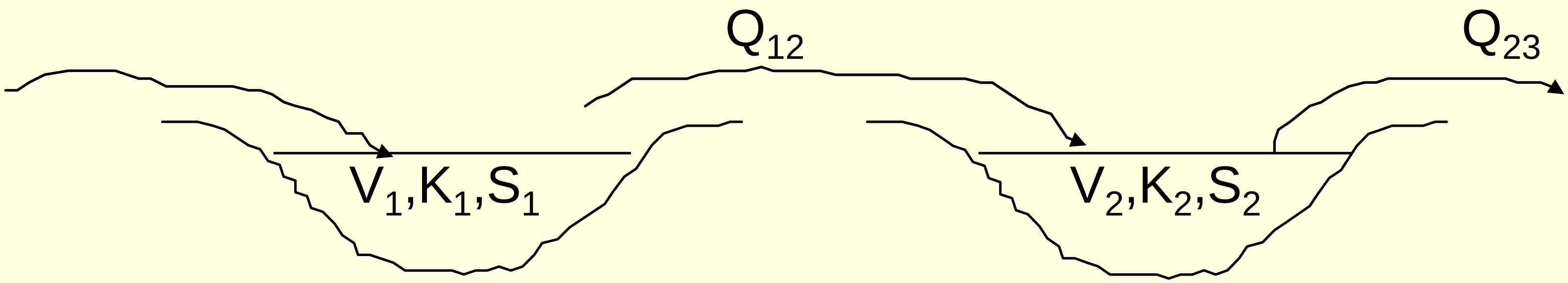
$$\left(\frac{dC}{dt}\right) = \frac{1}{\theta}C_i - \frac{1}{\theta}C + (-kC)$$

$$\left(\frac{dC}{dt}\right) + \left(\frac{1}{\theta} + k\right)C = \frac{1}{\theta}C_i$$

$$\text{where}\left(\frac{1}{\theta} + k\right) = \text{Characteristic (eigen) function}$$

$$\frac{1}{\theta}C_i = \text{Loading function}$$

湖泊序列的線型模式分析
Modeling a Series of Lakes



$$V_1 \frac{ds_1}{dt} + (Q_{12} + V_1 K_1) s_1 = W(t)$$

or

$$\frac{ds_1}{dt} + \alpha_1 s_1 = X_1(t)$$

where

$$\alpha_1 = \frac{Q_{12}}{V_1} + K_1$$

$$X_1 = \frac{W_1}{V_1}$$

解析解
Analytical Solutions

Lake 1

$$s_1(t) = \int_0^t X_1(\tau) h_1(t-\tau) d\tau$$

$$= \int_0^t \frac{W_1}{V_1} e^{-\alpha_1 (t-\tau)} d\tau$$

$$= \frac{W_1}{V_1 \alpha_1} (1 - e^{-\alpha_1 t})$$

Lake 2

$$s_2(t) = \int_0^t X_2(\tau) h_2(t-\tau) d\tau$$

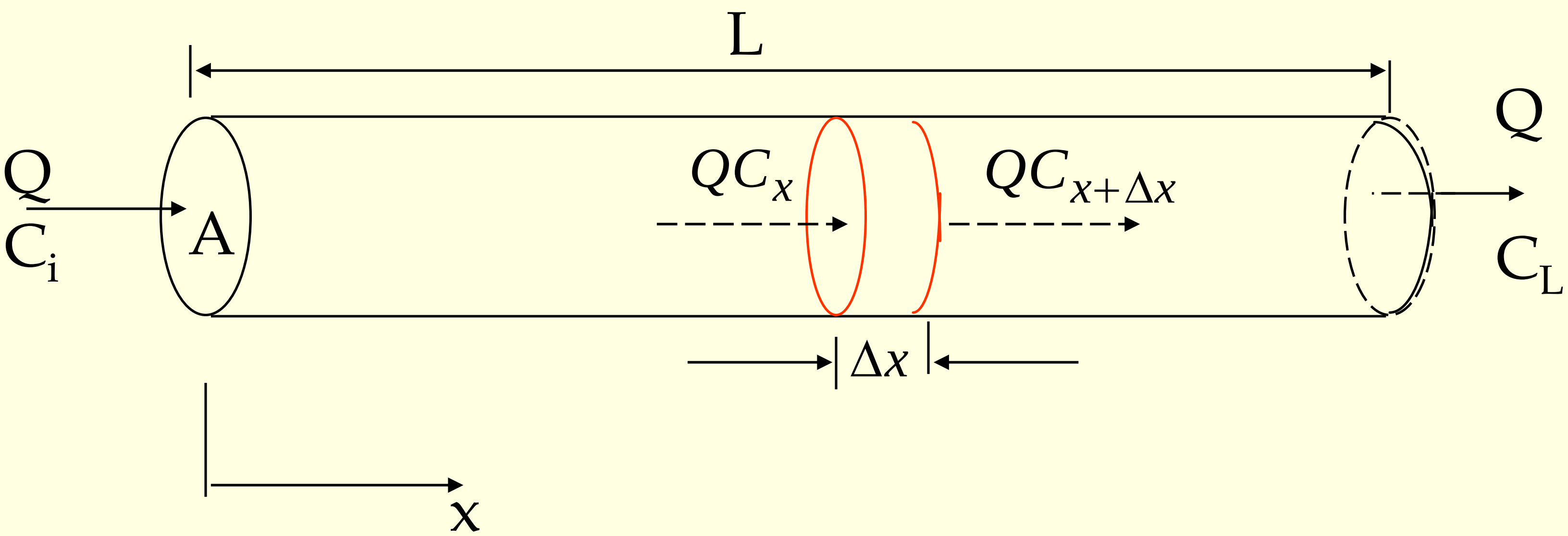
$$= \int_0^t \frac{Q_{12}}{V_2} s_1(\tau) h_2(t-\tau) d\tau$$

$$= \int_0^t \frac{Q_{12} W_1}{V_1 V_2 \alpha_1} (1 - e^{-\alpha_1 \tau}) e^{-\alpha_2 (t-\tau)} d\tau$$

$$= \frac{Q_{12} W_1}{V_1 V_2 \alpha_1} [\frac{1}{\alpha_2} (1 - e^{-\alpha_2 t}) - (\frac{e^{\alpha_2 t} - e^{\alpha_1 t}}{\alpha_2 - \alpha_1})]$$

B. 筒狀反應器

Plug-flow Reactor (PFR)



Mass balance equation for the incremental volume, $\Delta V = A\Delta x$:

$$\frac{d(A\Delta x)(C)}{dt} = QC_x - QC_{x+\Delta x} + (A\Delta x)r$$

筒狀反應器的數學模擬

Mathematical Model of a Plug-flow Reactor

Divide the equation by$(A\Delta x)$, and let $\Delta x \rightarrow 0$

$$\frac{dC}{dt} = \frac{Q}{A} \lim_{\Delta x \rightarrow 0} \left(\frac{C_x - C_{x+\Delta x}}{\Delta x}\right) + r$$

or

$$\frac{\partial C}{\partial t} = -\left(\frac{Q}{A}\right)\left(\frac{\partial C}{\partial x}\right) + r$$

Note that $u = \text{velocity} = Q/A$, therefore

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + r$$

筒狀模式在穩定狀態和一階反應下的解析解
Steady-state Plug-flow Model, with a First-order Reaction

Under steady – state conditions, $\frac{\partial C}{\partial t} = 0$, and

$$u\frac{dC}{dx} = r$$

Assume the reaction is a first - order decay, or $r = -kC$

then, $u\frac{dC}{dx} = -kC$

Introduce the boundary condition : $C = C_i$ at $x = 0$

$$C(x) = C_i e^{-(k\frac{x}{u})}$$

At the exit, $x = L, C = C^*$ and $C^* = C_i e^{-(k\frac{L}{u})} = C_i e^{-k\theta}$

where θ = mean hydraulic residence time

$$\theta = \frac{1}{k}\ln(\frac{C_i}{C^*})$$

例題: 應用穩定態筒狀反應器模式於河川水質分析

Application of Steady-state Plug Flow Reactor to River water Quality Analysis

Model Formulation

$$u\frac{dC}{dx} = r$$

For river modeling,

$$\mathrm{C} = \mathrm{D(DO\ deficit)}, \frac{\mathrm{d}x}{\mathrm{u}} = d\theta, r = k_1 L - k_2 D$$

$$So, \frac{dD}{d\theta} = k_1 L - k_2 D$$

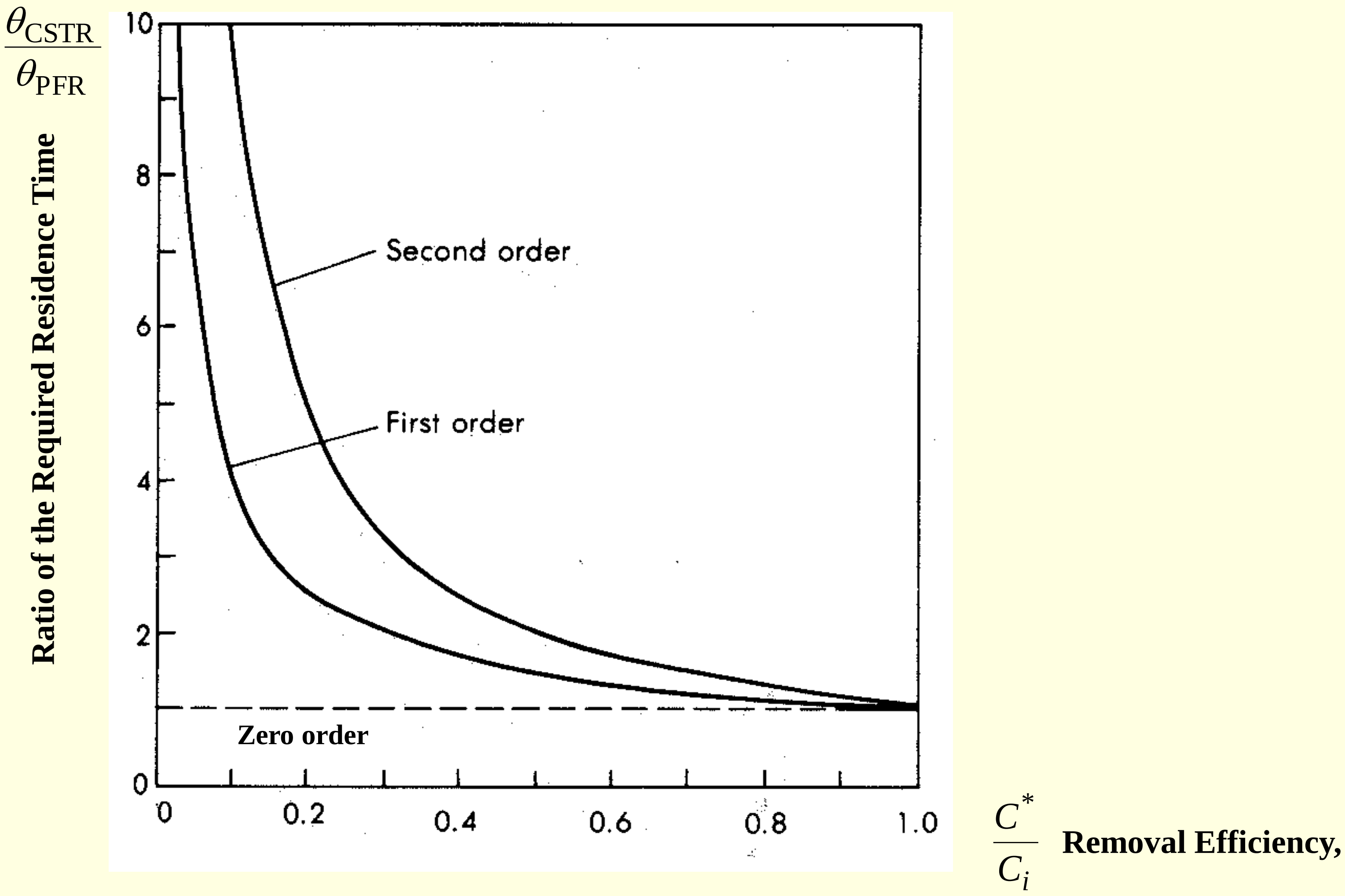
Boundary conditions: $\theta = 0$, $D = D_0$ and $L = L_0$

Model Solution

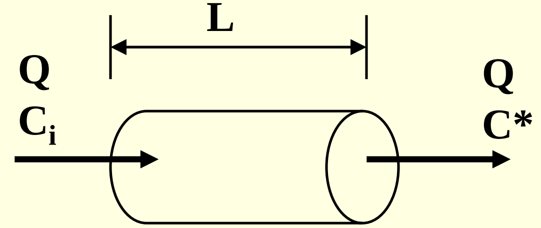
$$\mathrm{D}(\theta) = \frac{k_1 L_0}{k_2 - k_1}[\exp(-k_1\theta) - \exp(-k_2\theta)] + D_0 \exp(-k_2\theta)$$

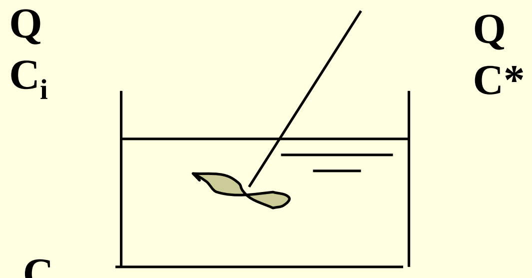
Streeter-Phelps model takes a receiving river as an ideal plug flow reactor in steady-state,

Performance Comparison of CSTRs and PFRs

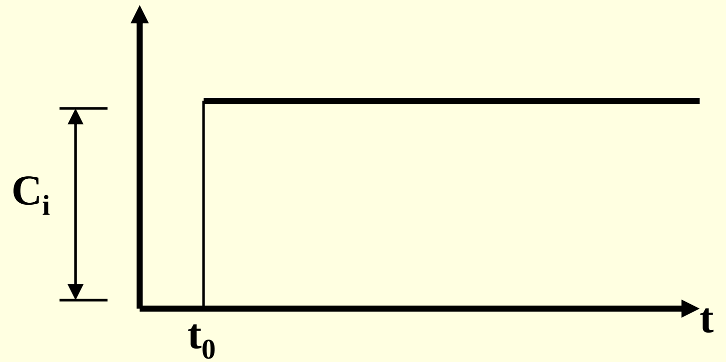


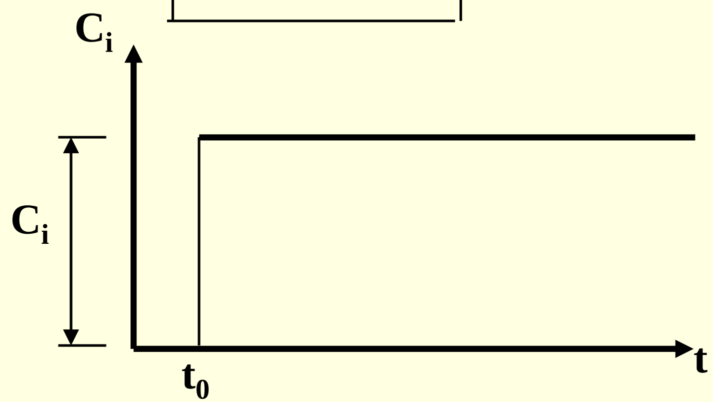
System Response of a CSTR and PFR Reactors to a Continuous, Constant, Conservative Tracer



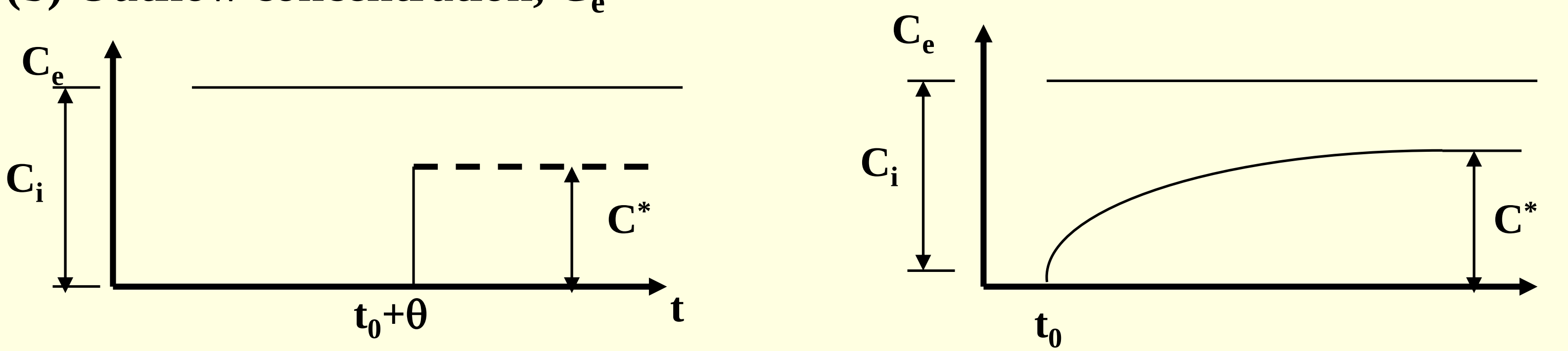


(a) Inflow concentration, C_i



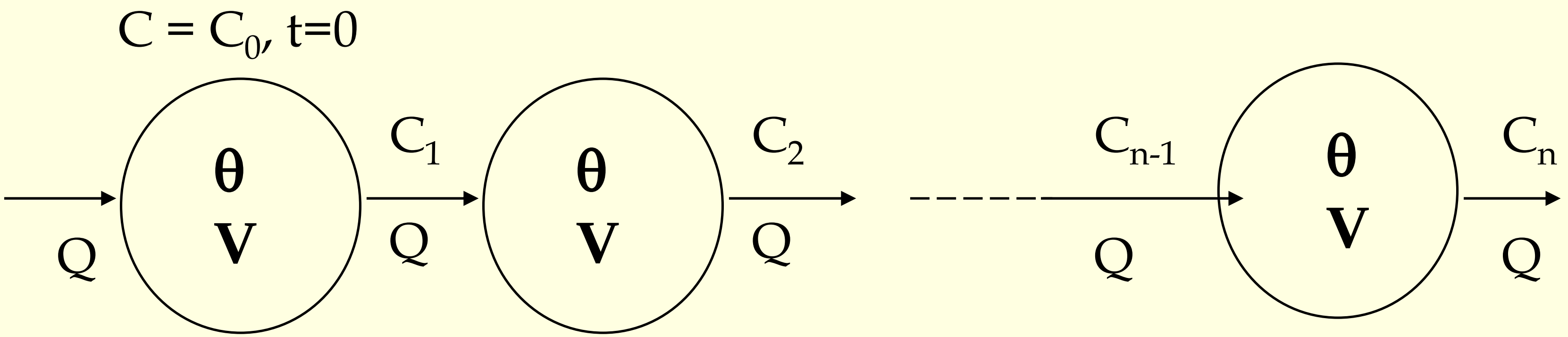


(b) Outflow concentration, C_e



C. 序列完全混合模式
Cascade of Complete-mix Reactors

Time-variable Solution with a Pulse Input of a Conservative Chemical(C_i = 0, k = 0, and $C = C_0$ at t = 0)



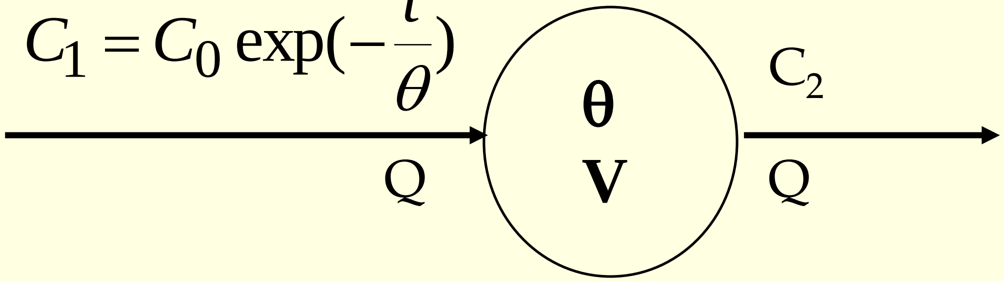
Concentration of the effluent from the first reactor:

$$C_1 = C_0 \exp\left(-\frac{t}{\theta}\right)$$

$$\text{where } \theta = \frac{V}{Q}$$

Determination of Effluent Concentration from Reactor 2

$$C_1 = C_0 \exp(-\frac{t}{\theta})$$



$$\frac{dC_2}{dt} = \frac{1}{\theta}(C_1 - C_2)$$

or

$$\frac{dC_2}{dt} + \frac{1}{\theta} C_2 = C_0 \frac{1}{\theta} \exp(-\frac{t}{\theta})$$

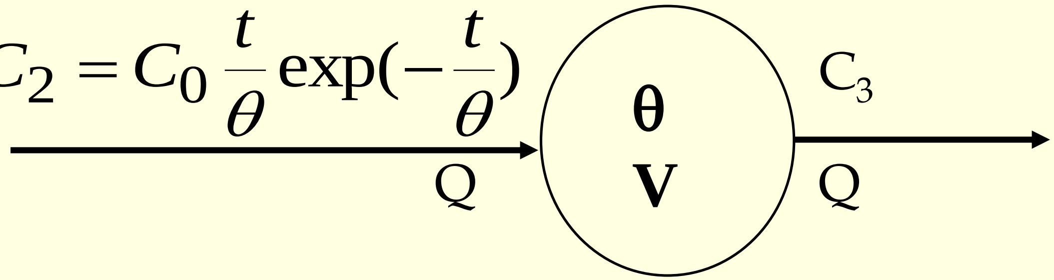
Solution with the initial condition, $C_2 = 0$ at t = 0

by the method of integrating factor

$$C_2 = C_0 \frac{t}{\theta} \exp(-\frac{t}{\theta})$$

Determination of Effluent Concentration from Reactor 3

$$C_2 = C_0 \frac{t}{\theta} \exp(-\frac{t}{\theta})$$



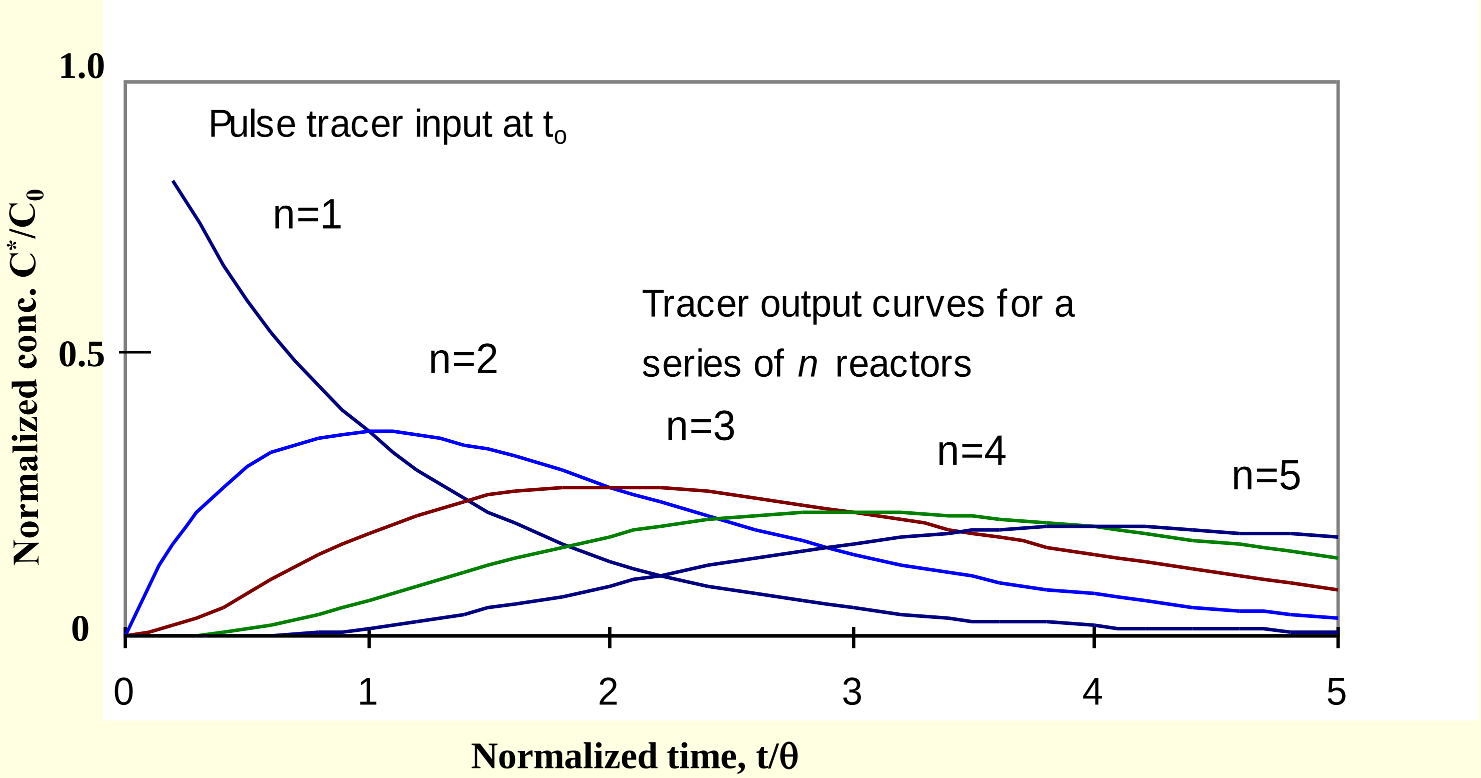
$$\frac{dC_3}{dt} = \frac{1}{\theta}(C_2 - C_3)$$

$$\frac{dC_3}{dt} + \frac{1}{\theta} C_3 = C_0 (\frac{t}{\theta^2}) \exp(-\frac{t}{\theta})$$

Solution with the initial condition $, C_3 = 0 \; at \; t = 0$

$$C_3 = \frac{1}{2} C_0 (\frac{t}{\theta})^2 \exp(-\frac{t}{\theta})$$

Performance of a series of Complete-mix Reactors in a series

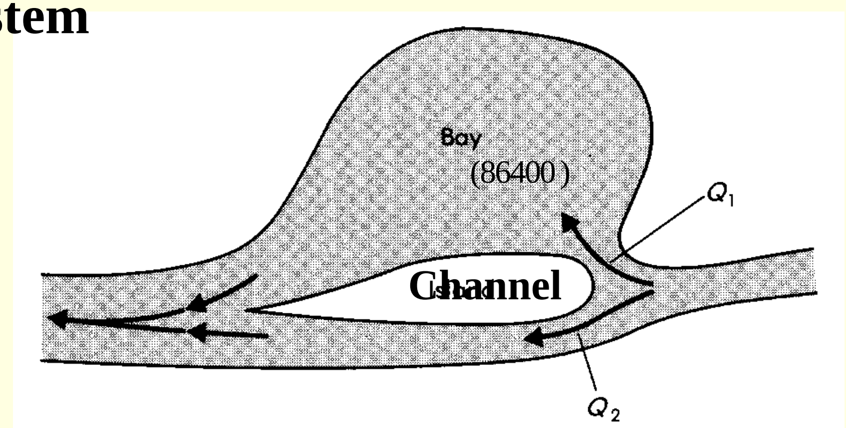


例題：理想反應器模擬複雜河川系統

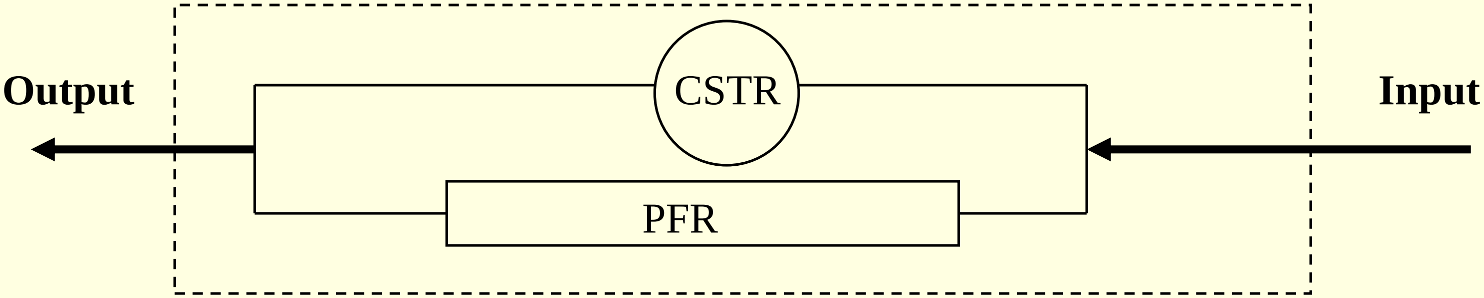
Mathematical Model of a River-Channel System by a Combination of CSTR and PFR

A river is split by an island with part of the flow remaining in a narrow channel and the remainder flowing into a bay before returning to the main channel as shown above. Based on dye studies it was found that the bay behaves as a CSTR of volume 3.14 x 106 m^3. And the channel behaves as a PFR of length 2500 m, depth 2m, and width 30 m. When the total flow is 28 m^3/sec it is divided as Q1 = 12 m3/sec and Q2 = 16 m3/sec. If the dye is added above the junction to give an initial concentration of 10 g/m^3 that extended over 280 m^3,determine the ideal response curve below the point the stream join.

River-Bay System



Model



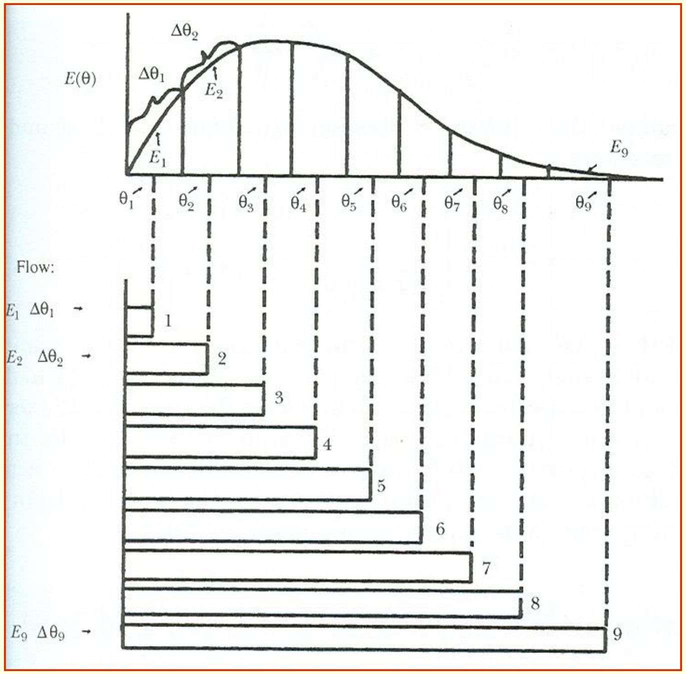
D. 非理想反應器的模式分析

Non-ideal Reactors Segregated-Flow Model (SFM)

The SFM is obtained by approximating the real reactors as numerous plug flow reactors that have difference residence time and exit age characteristics.

The performance of the reactor can be determined by the following equation:

$$\frac{\overline{C}}{C_0} = R(\theta_1)E_1\Delta\theta_1 + R(\theta_2)E_2\Delta\theta_2 + \ldots + R(\theta_i)E_i\Delta\theta_i$$



C_0 = influent concentration, mg/L

$\overline{C}$ = average effluent concentration, mg/L

θ_i = exit age $(t/t_R)_i$ for fluid element i

E_i = exit age distribution for fluid element i

$E_i\Delta\theta_i$ = fraction of exit stream that has age θ_i

$R(\theta_i)$ = dimensionless effluent concentration with hydraulic residence time that corresponds to θ_i

For first-order reaction: $R(\theta) = \exp(-k\theta t_R)$

Example Application of SFM to model a disinfection system

A disinfection study was conducted in a laboratory batch reactor and the Ct value required to accomplish a 99.99 percent reduction (4 log removal) in the target organism was determined. A full-scale disinfection contactor was then designed to accomplish 4 log removal of the target organism based on the laboratory results [i.e., the product of the residual concentration and hydraulic residence time ($C\tau$) was set equal to the Ct value for 4 log removal determined in the batch study].

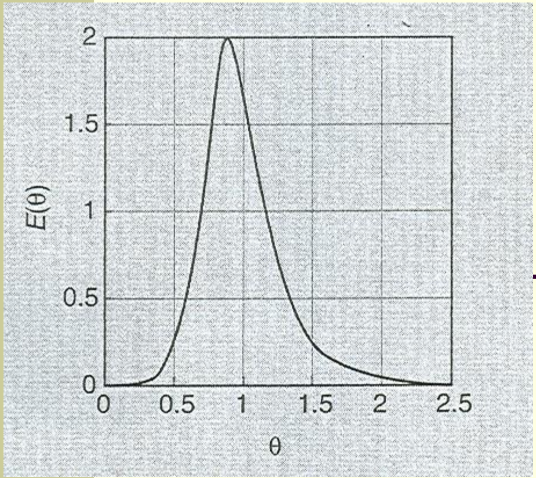
After the full-size contactor was built, tracer tests were conducted to evaluate the hydraulic characteristics of the contactor. Using the procedures outlined in last slide, the tracer curve has been analyzed to produce the exit age distribution. The results of the tracer study are given in the following table:

θ	$E(\theta)$	θ	$E(\theta)$	θ	$E(\theta)$
0.15	0	0.91	1.541	1.67	0.067
0.31	0.017	1.06	0.928	1.82	0.046
0.46	0.279	1.21	0.446	1.98	0.036
0.61	0.895	1.36	0.251	2.13	0.015
0.76	1.995	1.52	0.128	2.28	0

Using the tracer study data and contactor design information: (a) plot the exit age distribution $E(\theta)$ versus θ; (b) develop an equation for $R(\theta)$ as a function of θ and assume that $\log[R(\theta)]$ varies linearly with changes in θ and that, when $\theta = 0$, $R(\theta) = 1$; and (c) use $E(\theta)$, $R(\theta)$, and the SFM model to estimate the level of inactivation, $\log(N/N_o)$, that will actually occur in the full-scale reactor with dispersion.

Solution

1. Plot the exit age distribution using the data provided in the problem statement. The exit age distribution is plotted below:



Solution

1. Plot the exit age distribution using the data provided in the problem statement. The exit age distribution is Shown in the left.

   Using information provided in the problem statement, determine the form of the $R(\theta)$ function.

   a. From the definition of θ, when $t = \tau$, $\theta = 1$. Further, when $t = \tau$, the removal is 99.99 percent. Therefore, $R(1) = 10^{-4}$.

   b. From the definition of θ, when $t = 0$, $\theta = 0$, therefore $R(0) = 1$.

   c. As given in the problem statement, $\log[R(\theta)]$ varies linearly with θ; thus the following relationship is obtained:

$$\log[R(\theta)] = s\theta$$

where s = slope of linear relationship between $\log[R(\theta)]$ and θ

   d. When $R(\theta)$ is plotted as a function of θ on a semi-log plot, $s = -4$, and the following equation is obtained for $R(\theta)$:

$$\log[R(\theta)] = -4\theta \qquad R(\theta) = 10^{-4\theta}$$

2. Determine the degree of inactivation achieved with the contactor.

   a. Using the data given in the problem statement, a numerical solution may be obtained using the following summation form of Eq. 6-157:

$$\frac{N}{N_o} \cong \sum_{\theta=0}^{\theta=\infty} E[\theta]R[\theta]\, d\theta = \sum_{\theta=0}^{\theta=\infty} E[\theta]10^{-4\theta}\, d\theta$$

   b. The necessary calculations in tabular form are as follows:

θ	$E(\theta)$	$R(\theta)$	$d\theta$	$R(\theta)E(\theta)\ d\theta$
0.00	0	0		
0.15	0	2.45E-01	0.15	0.00
0.31	0.017	6.00E-02	0.16	1.55×10^{-4}
0.46	0.279	1.47E-02	0.15	6.26×10^{-4}
0.61	0.895	3.61E-03	0.15	4.93×10^{-4}
0.76	1.995	8.84E-04	0.15	2.69×10^{-4}
0.91	1.541	2.36E-04	0.14	5.22×10^{-5}
1.06	0.928	5.79E-05	0.15	8.21×10^{-6}
1.21	0.446	1.42E-05	0.15	9.67×10^{-7}
1.36	0.251	3.48E-06	0.15	1.33×10^{-7}
1.52	0.128	8.52E-07	0.16	1.67×10^{-8}
1.67	0.067	2.09E-07	0.15	2.13×10^{-9}
1.82	0.046	5.12E-08	0.15	3.61×10^{-10}
1.98	0.036	1.25E-08	0.16	6.88×10^{-11}
2.13	0.015	3.07E-09	0.15	7.22×10^{-12}
2.28	0	7.53E-10	0.15	0.00
				$\Sigma = 0.00160$

c. The degree on inactivation is

$$\log\left(\frac{N}{N_o}\right) = -\log(0.00160) = 2.79$$

Comment

The performance of the full-scale contactor has been reduced from a theoretical value determined in the laboratory of 4 logs to less than 3 logs of inactivation due to the dispersion.