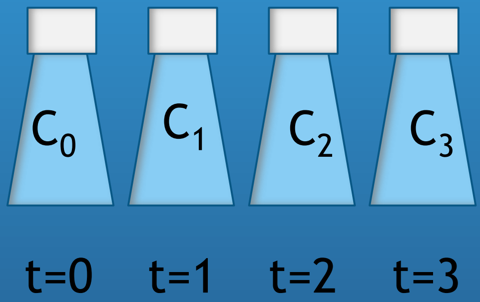
污染物在河川之傳輸

閱讀資料:劉成均,水質模式分析, 2016(pp.3-1~3-29)

Reaction Kinetics of Pollutants in rivers

- A simple experiment to collect rate data for a pollutant in nature water (e.g. River)



Time	0	1	2	3
Concentration	c0	c1	c2	c3

Reaction Kinetics

$$\frac{dc_A}{dt} = -kf(c_A, c_{B,}....)$$

$$\frac{dc}{dt} = -kc^n$$

C= concentration
n= order
K=temperature-dependent concentration

Reaction Kinetics

$$\frac{dc}{dt} = -kc^n$$

C= concentration
n= order
K=temperature-dependent concentration

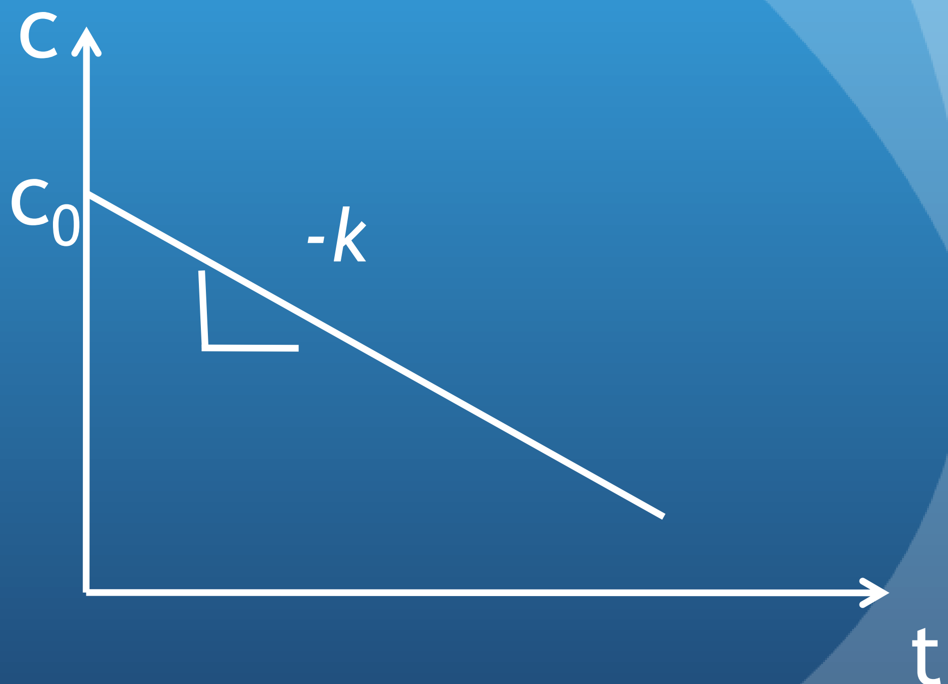
n=0 zero-order
n=1 first-order
n=2 second-order

Reaction Kinetics

n=0 zero-order

$$\frac{dc}{dt} = -k$$

$$c = c_0 - kt$$



C= concentration
n= order
K=temperature-dependent constant

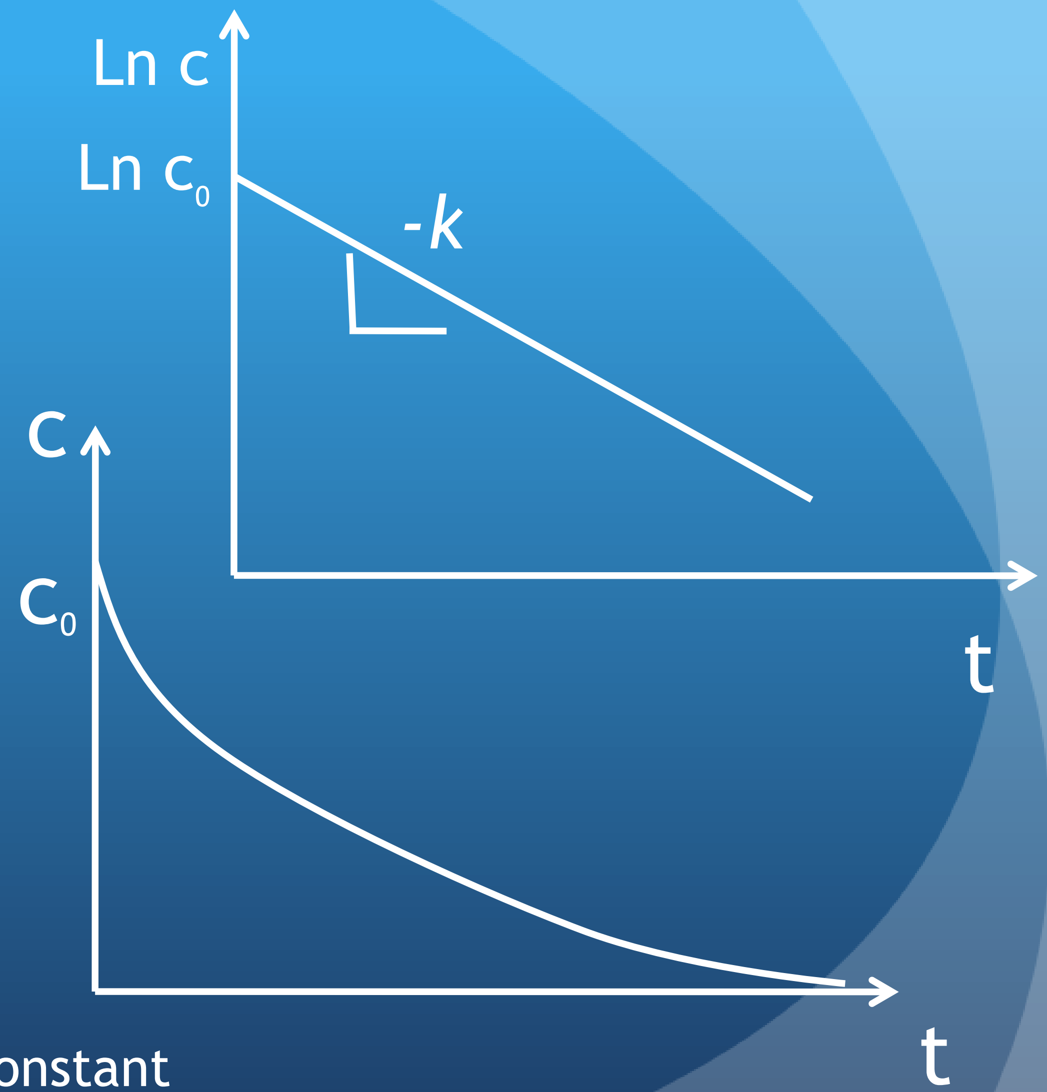
Reaction Kinetics

n=1 first-order

$$\frac{dc}{dt} = -kc$$

$$\ln c - \ln c_0 = -kt$$

C= concentration
n= order
K=temperature-dependent constant

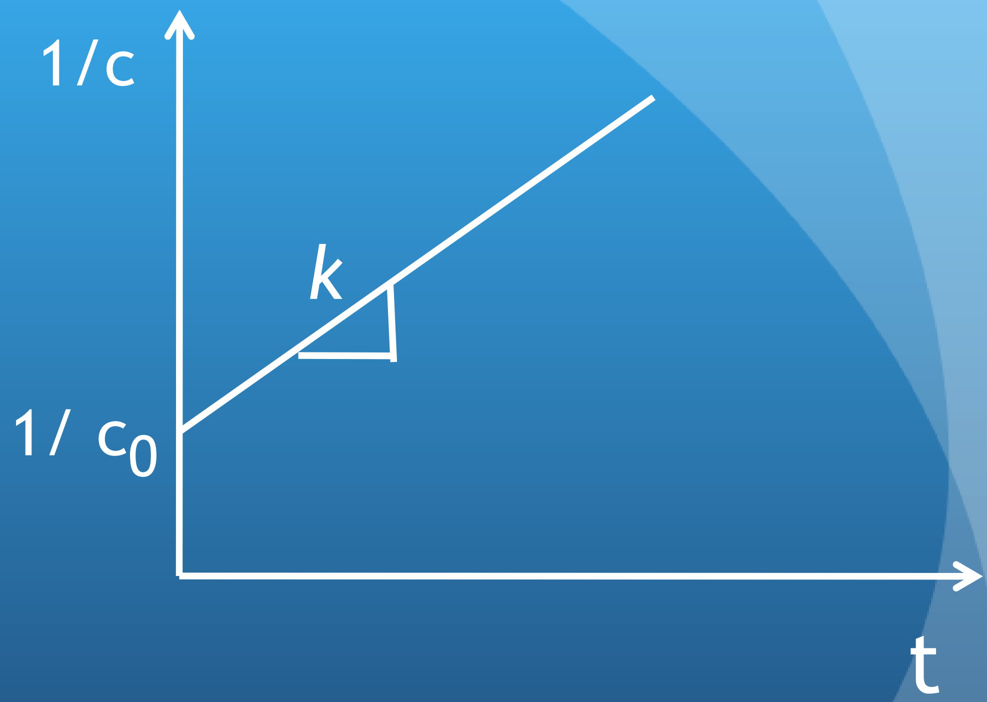


Reaction Kinetics

n=2 second-order

$$\frac{dc}{dt} = -kc^2$$

$$\frac{1}{c} = \frac{1}{c_0} + kt$$



C= concentration
n= order
k=temperature-dependent constant

Reaction Kinetics

The integral Method

order	Rate units	Dependent (y)	Independent (x)	intercept	slope
zero	$M(L^3T)^{-1}$	c	t	c_0	-k
first	T^{-1}	lnc	t	$\ln c_0$	-k
second	$L^3(MT)^{-1}$	1/c	t	$1/c_0$	k
general	$(L^3M^{-1})n^{-1}T^{-1}$	C^{1-n}	t	C_0^{1-n}	(n-1)k

Example

- Employ the integral method to determine whether the following data is zero-, first-, or second-order:

t(d)	0	1	3	5	10	15	20
c(mg/L)	12	10.7	9	7.1	4.6	2.5	1.8

Effects of Temperature on Reaction Rate

$$\frac{k(T_2)}{k(T_1)} = \theta^{T_2 - T_1}$$

$$k(T) = k(20)\theta^{T-20}$$

K=temperature-dependent constant

T_1, T_2=temperature (^oC)

θ	Reaction
1.024	Oxygen reaeration
1.047	BOD decomposition
1.066	Phytoplankton growth
1.08	Sediment oxygen demand(SOD)

Example

A laboratory provides you with the following results for a reaction:

$T1=4\ ^oC$, $k1=0.12d^{-1}$

$T2=16\ ^oC$, $k2=0.20d^{-1}$

(a) Evaluate θ for this reaction

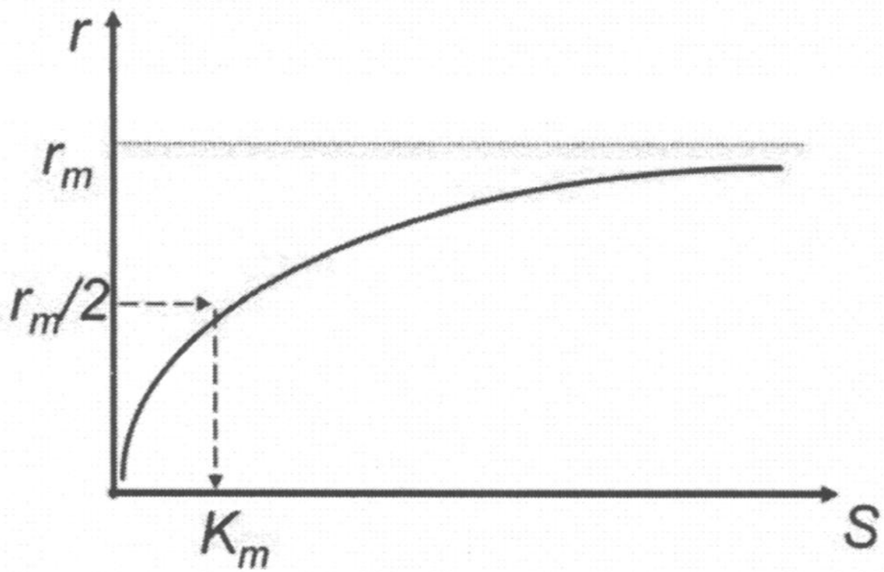
(b) Determine the rate at 20 ^oC

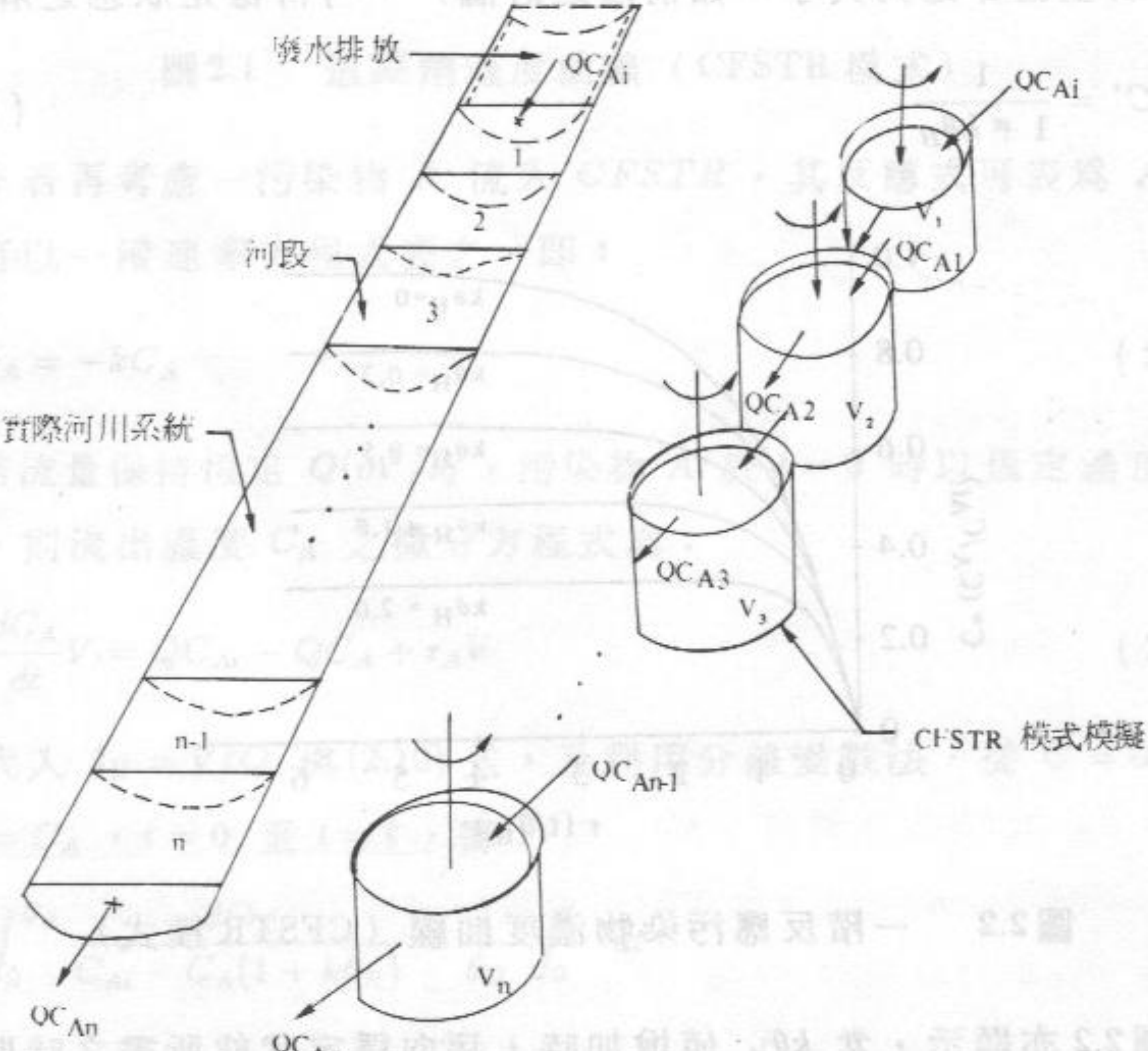
Reaction Kinetics

- Michaelis-Menten enzyme kinetics

$$r = \frac{dS}{dt} = \frac{r_m S}{K_m + S}$$

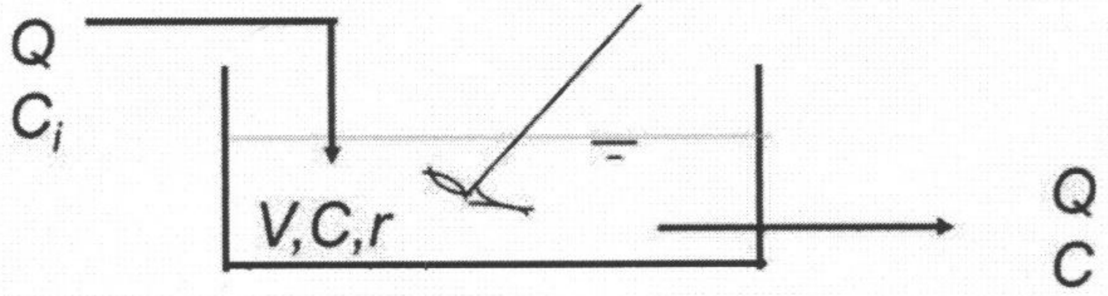
r_m = Maximum reaction rate constant
K_m = half-saturation constant
S= Substrate concentration





廢水排放
QC_Ai
1
2
河段
3
實際河川系統
n-1
n
QC_An
QC_An
V_n
QC_An-1
QC_Ai
V_1
QC_A1
QC_A2
V_2
QC_A3
V_3
CFSTR 模式模擬

Complete-mix reactor or Completely Stirred Tank Reactor (CSTR)



Mass Balance Principle:
Rate of Accumulation = Mass Flux In - Mass Flux Out + Reaction Rate

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

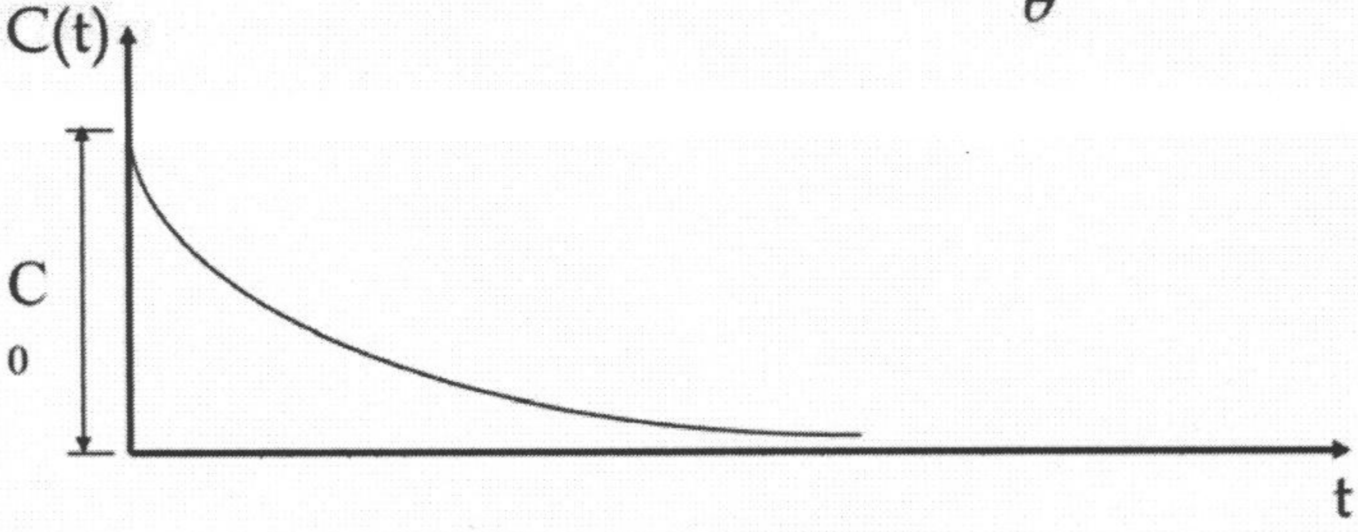
For a first – order reaction, $r = -kC$ then,

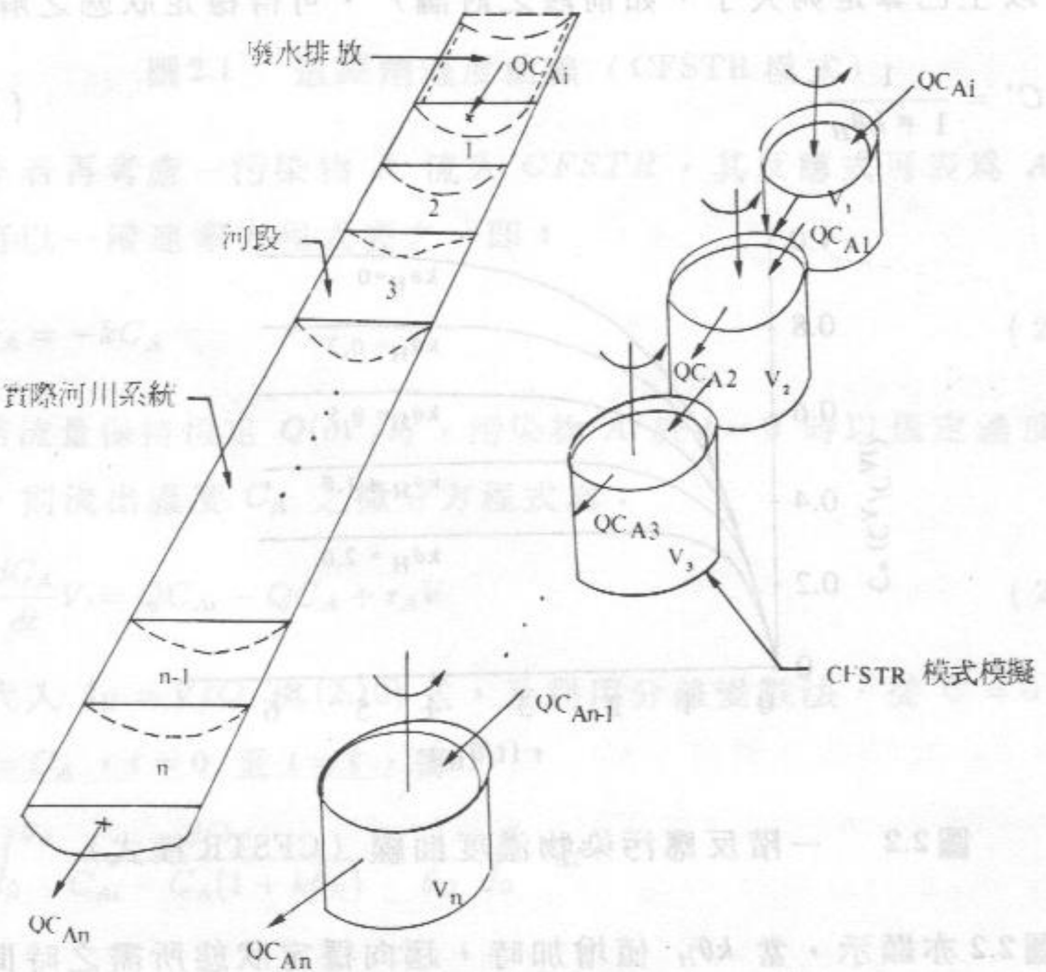
$$V(\frac{dC}{dt}) = QC_i - QC + V(-kC)$$

CSTR with Pulse Input

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

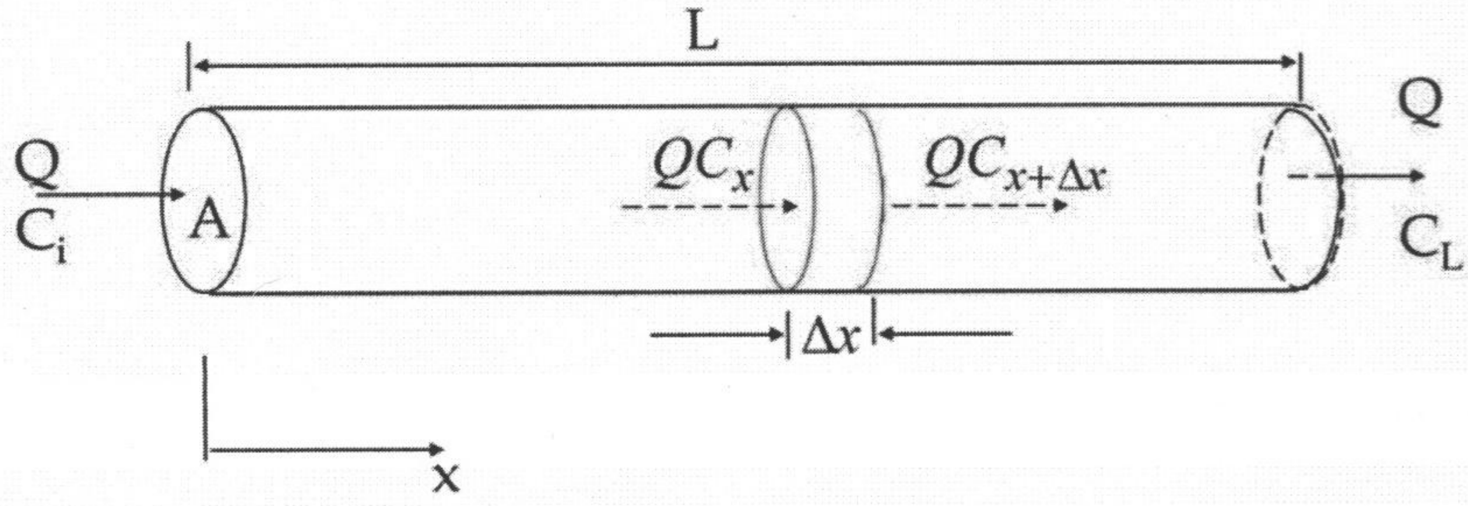
$$or, C(t) = C_0 \exp[-(\frac{1}{\theta} + k)t]$$





$$C_{An} = C_{Ai}\left(\frac{1-e^{-(1+k\theta_{H_1})\tau_1}}{1+k\theta_{H_1}}\right)\left(\frac{1-e^{-(1+k\theta_{H_2})\tau_2}}{1+k\theta_{H_2}}\right)\cdots\left(\frac{1-e^{-(1+k\theta_{H_n})\tau_n}}{1+k\theta_{H_n}}\right)$$

Plug-flow reactor



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

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