Session 3: Mathematical Formulation and Application of River Water Quality Models

第一單元: 河川水質模式的建立和應用

1. 河川簡易水質模式的介紹和討論
   Simple River Water Quality Modeling

2. 河川複雜水質模式的介紹和討論
   Comprehensive River Water Quality Modeling

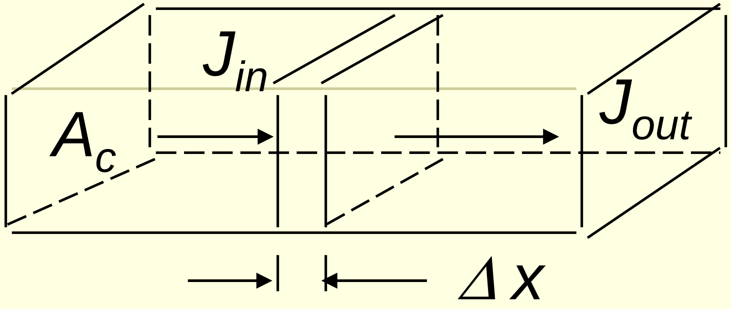
3. 污染物在河川內傳輸機制及數學模擬和模式係數值估算
   Reaction Kinetics of Pollutants in Rivers

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

1. 河川簡易水質模式的介紹和討論

Simple River Water Quality Modeling

A. Streeter-Phelps Model for Non-Tidal River



$$Continuity\ Equation: \frac{\partial C}{\partial t} + \frac{\partial J}{\partial x} = r$$

$$J = Mass\ flux = Advective\ Flux + Dispersive\ Flux$$

$$Advective\ Flux = UC$$

$$Dispersive\ Flux = -E\frac{\partial C}{\partial x}\quad (E = dispersion\ coefficient)$$

$$So,\ \frac{\partial C}{\partial t} - E\frac{\partial^2 C}{\partial x^2} + U\frac{\partial C}{\partial x} = r$$

Deriving the Streeter-Phelps Equation by Simplifying a One-Dimensional Transport Model

Use DO Deficit D as the dependent variable,

one-dimensional transport equation becomes,

$$\frac{\partial D}{\partial t} - E\frac{\partial^2 D}{\partial x^2} + U\frac{\partial D}{\partial x} = r$$

Simplifying Assumptions:

(1) Non-dispersive, or $E = 0$

(2) Steady-state, or $\frac{\partial D}{\partial t} = 0$

(3) Two reactions of deoxygenation and reaeration, or

$r = k_1 L - k_2 D$, Then

$$U\frac{dD}{dx} = k_1 L - k_2 D \quad \text{or} \quad \frac{dD}{d\theta} = k_1 L - k_2 D$$ → Streeter-Phelps Model

where θ is the time of travel, or $\theta = x/U$

Solution of the Streeter-Phelps Model

Streeter-Phelps model can also be formulated directly by taking a receiving river as **an ideal plug flow reactor under steady-state**,

Mathematical Model

$$\frac{dD}{d\theta} = r$$

$$\text{Note that } r = k_1 L - k_2 D \text{ or, } \frac{\mathrm{d}D}{\mathrm{d}\theta} = k_1 L - k_2 D$$

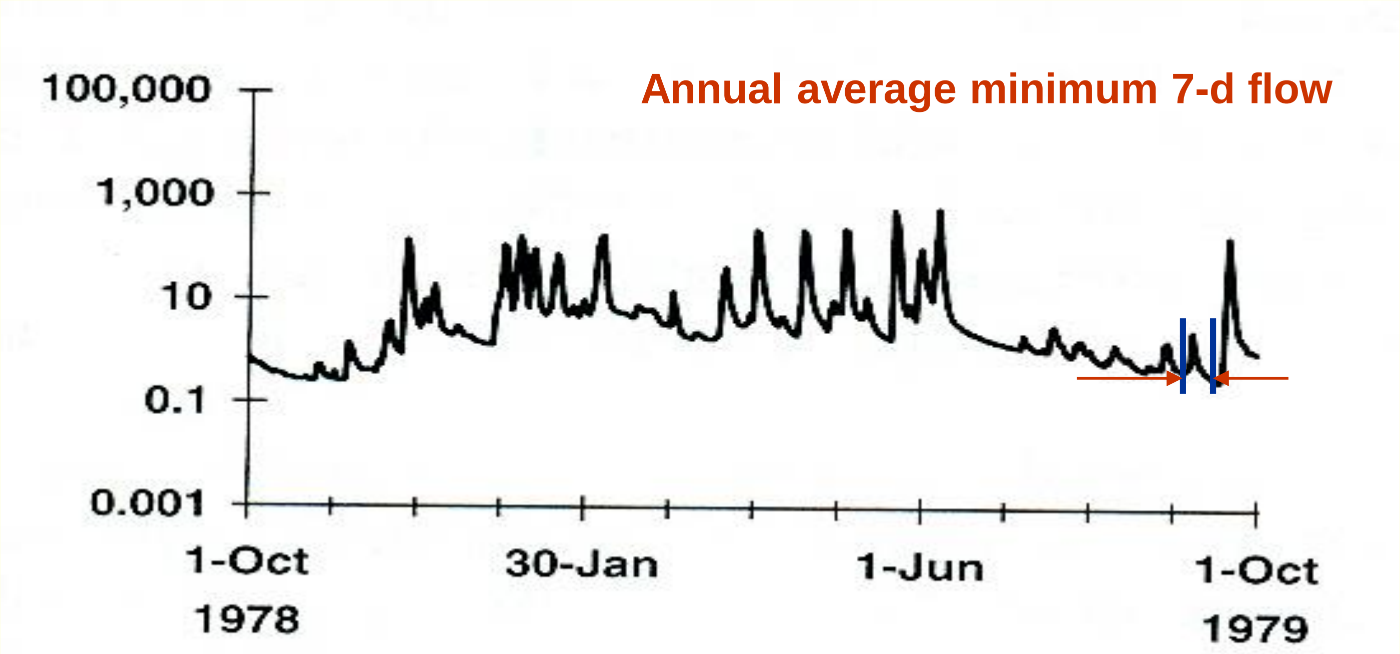
$$\text{Boundary conditions}: \theta = 0,\ \mathrm{D} = \mathrm{D}_0 \text{ and } \mathrm{L} = \mathrm{L}_0$$

Model Solution

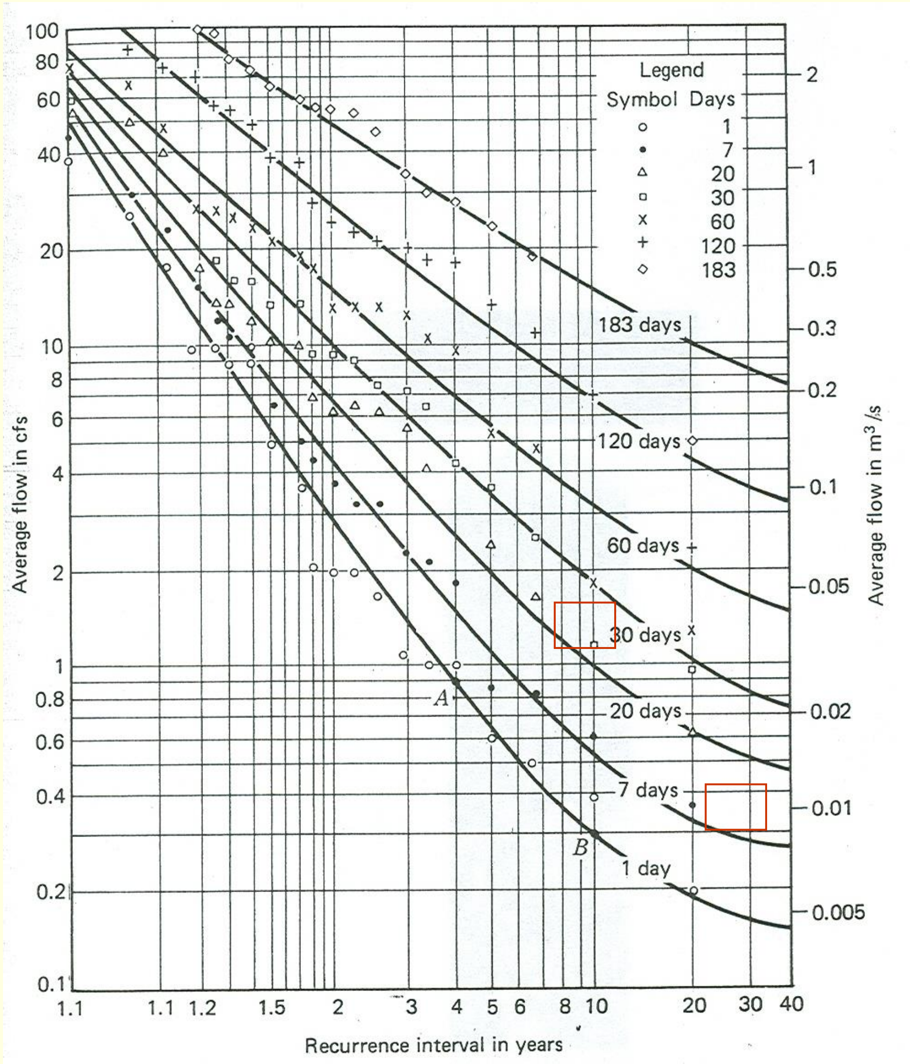
$$\mathrm{D}(\theta) = \frac{\mathrm{k}_1 \mathrm{L}_0}{\mathrm{k}_2 - \mathrm{k}_1}[\exp(-\mathrm{k}_1\theta) - \exp(-\mathrm{k}_2\theta)] + \mathrm{D}_0 \exp(-\mathrm{k}_2\theta)$$

Streeter-Phelps Model and Low flow Analysis

IN USA, waste load allocation using Streeter-Phelps model has been conducted under the design flow conditions of MA7CD10, or a minimum 7-d flow with a recurrence interval of 10 years in the receiving river

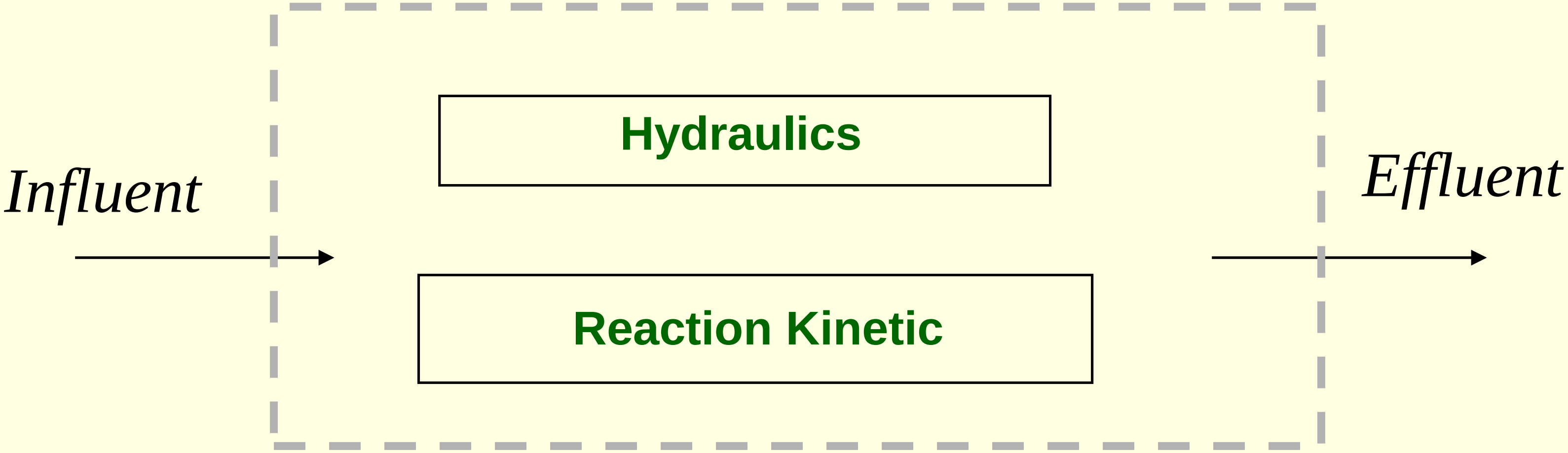


Frequency of minimum flows for Yellow Creek near Hammondsville, Ohio (1915-1935)



Transport and Reaction Mechanisms in a Streeter-Phelps Model

Environment Transport System


Influent

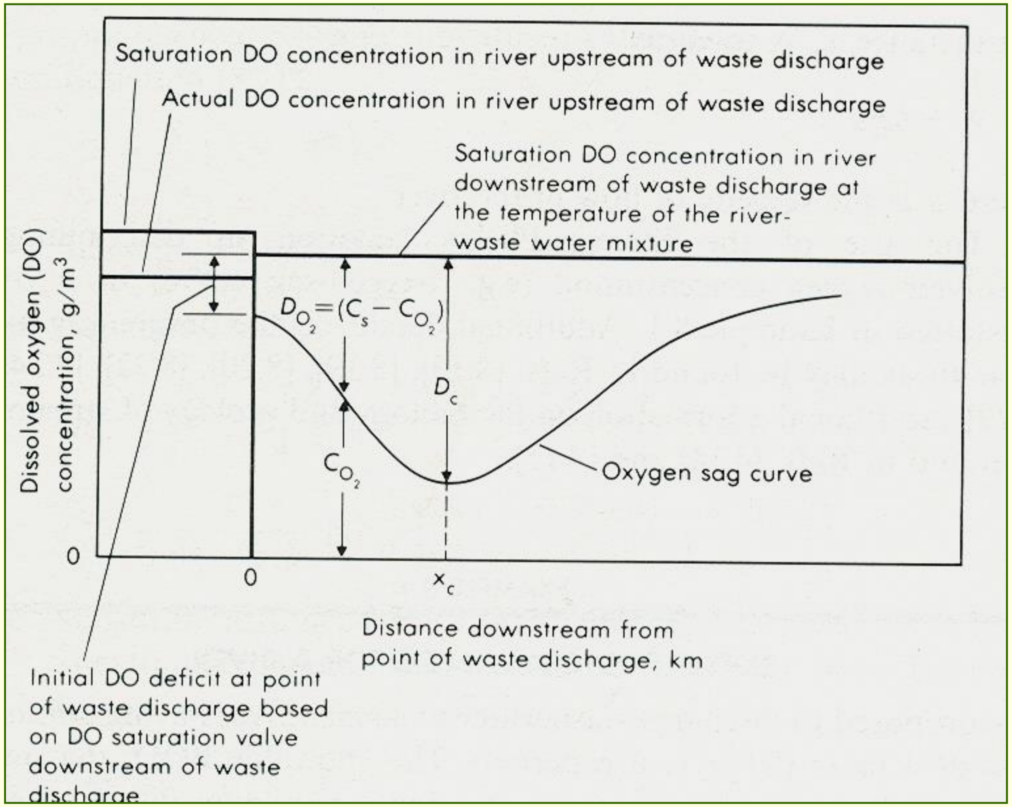
Hydraulics

Reaction Kinetic

Effluent

(1) One Hydraulic (Transport) Mechanism: travel time: $\theta = x/u$, u is the stream velocity.
(2) Two reaction mechanisms: (a) Deoxygenation rate: k_1L ; (b) Reaeration rate: k_2D

Critical Point in a DO Sag Curve



$$\theta_c = \frac{1}{k_2 - k_1} \ln\left[\frac{k_2}{k_1}\left(1 - D_0 \frac{k_2 - k_1}{k_1 L_0}\right)\right]$$

$$D_c = \frac{k_1}{k_2} L = \frac{k_1}{k_2} L_0 \exp(-k_1 \theta_c)$$

1. 河川簡易水質模式的介紹和討論

B. Flushing Time Model for Estuaries and Tidal Rivers

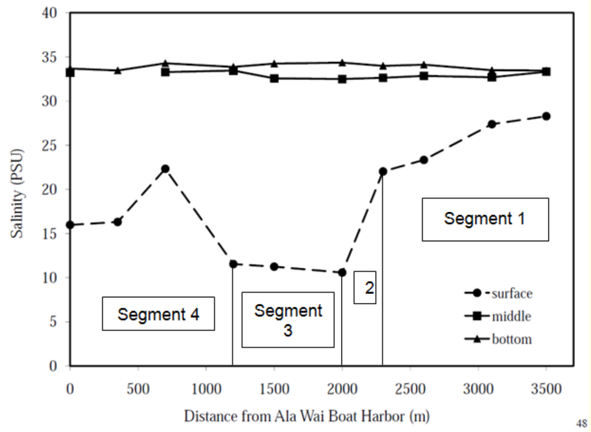
In calculating the waste assimilative capacity of an estuary, one of the most important factors is the estuary’s flushing time. Flushing time is defined as the length of time required to replace the existing fresh water in an estuary at a rate equal to the river discharge. In other words, flushing time represents the average time that a particle spends within the estuary based on its input position.

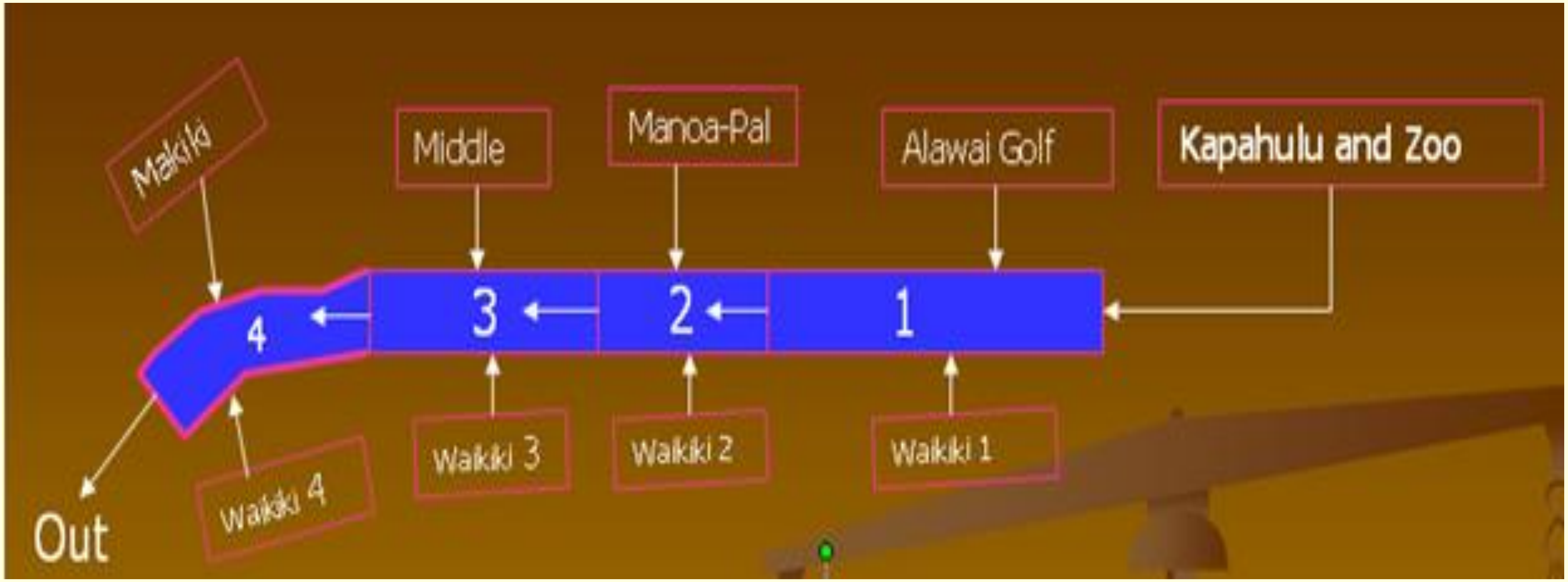
A simple estuary water quality model can be formulated based on the fraction of freshwater method given in an EPA Water Quality Assessment report of 1977

Demonstration on the fraction of Freshwater Method

Water Quality Modeling of Ala Wai Canal on Oahu, Hawaii

Ala Wai Canal was simulated as a series of 4 CSTRs





Average Dry Season Salinity

Segment #	Surface	Half Meter	1 Meter	2 Meters	3 Meters	4 Meters
1	23.7	29.7	32.0	33.2	33.5	0
2	15.7	25	30.9	33.1	0	0
3	19.9	26.1	31.6	33.3	28.9	0
4	22.0	27.2	32	33.5	33.6	33.7

Average Wet Season Salinity

Segment #	Surface	Half Meter	1 Meter	2 Meters	3 Meters	4 Meters
1	25	26.6	28.9	33	33.4	0
2	17.9	21.4	27.6	32.1	0	0
3	16.4	22.2	28.6	33	26.7	0
4	17.9	23.6	30.3	33.4	33.5	33.5

Calculate Each Segment's Fraction of Freshwater

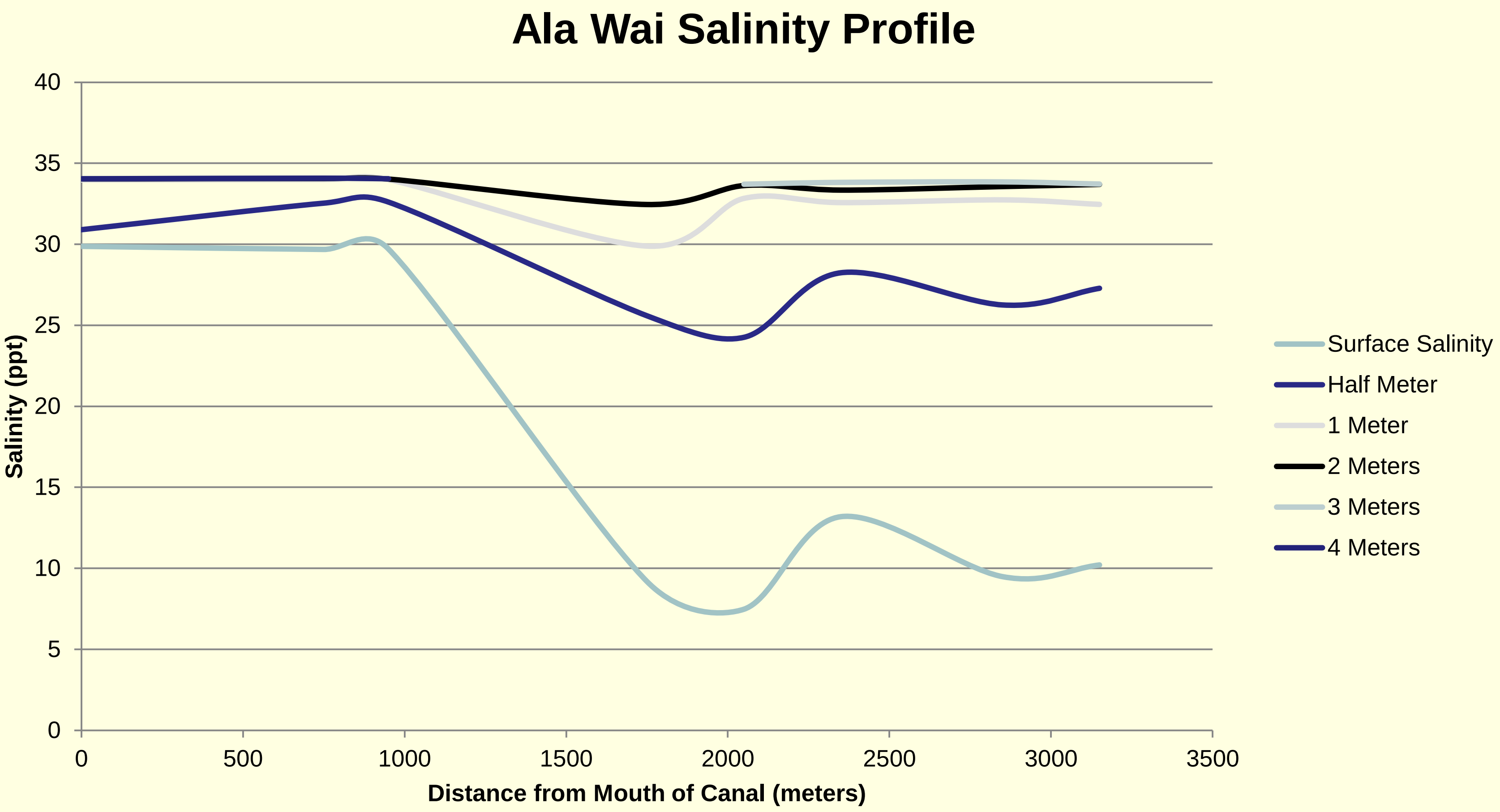
$$f_i = \frac{S_s - S_i}{S_s}$$

f_i = fraction of freshwater in segment "*i*"

S_s = salinity of sea water = 34.55 parts per thousand

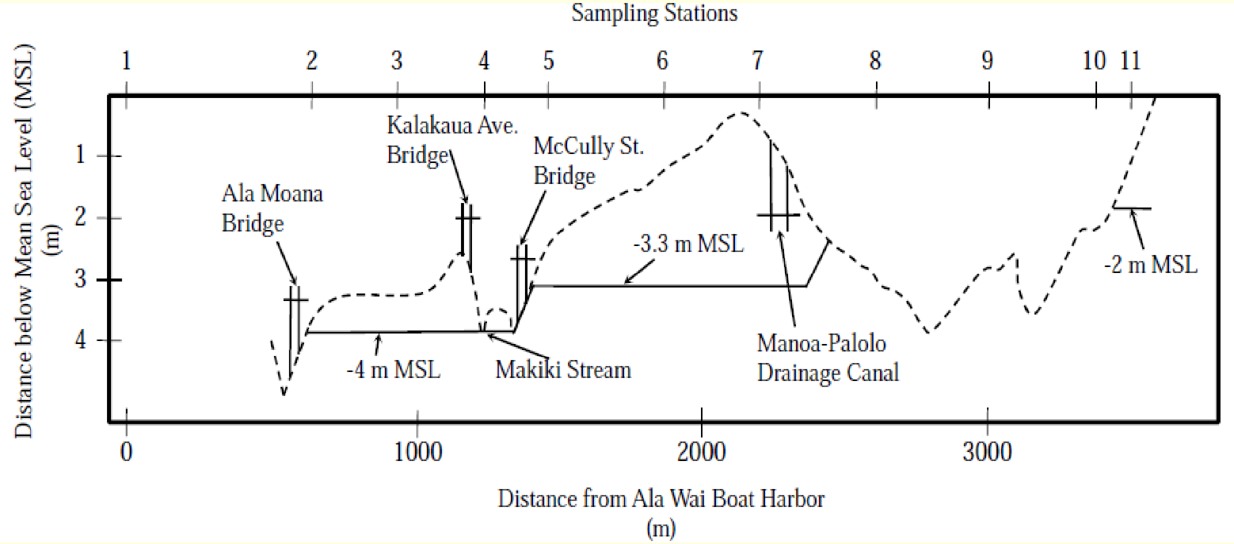
S_i = mean salinity for segment "*i*"

Graph the Salinity Profile



Calculate the Quantity of Freshwater in Each Segment

W_i = quantity of freshwater in segment "i" = f_i x volume of segment



Segment Number	Volume (m^3)	Dry Season Quantity of Freshwater (m^3)	Wet Season Quantity of Freshwater (m^3)
1	260,070	23018	32000
2	58,740	17695	20067
3	172,216	25006	36440
4	230,592	18735	25679

Calculate the Flushing Time for Each Segment

$$T_i = W_i/R$$

T_i = segment flushing time
R = total river discharge over one tidal cycle

- Example of *R*-value calculation for segment 1

$$12\text{cfs} \text{ x } \frac{0.283\text{cubic meters}}{1.0\text{ cubic feet}} \text{ x } \frac{3600\text{ seconds}}{\text{hour}} \text{ x } 12.4\text{ hours/tidal cycle}$$

Dry Season Flushing Times

Section	Freshwater Inputs	R-Value (m^3/tidal cycle)	Flushing Time (hours)
1	Golf, Waikiki 1, Zoo	13,110	21.77
2	Man-Pal, Waikiki 2	25,935	8.45
3	Middle, Waikiki 3	27,567	11.25
4	Makiki, Waikiki 4	35,551	6.53

- total calculated flushing time is 48.0 hours

Wet Season Flushing Times

Section	Freshwater Inputs	R-Value (m^3/tidal cycle)	Flushing Time (hours)
1	Golf, Waikiki 1, Zoo	15,172	26.15
2	Man-Pal, Waikiki 2	39,287	6.33
3	Middle, Waikiki 3	42,394	10.66
4	Makiki, Waikiki 4	68,734	5.39

Calculate the Flushing Time for Each Segment

$$T_i = W_i/R$$

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R = total river discharge over one tidal cycle

- example R-value calculation for segment 1

$$12\text{cfs} \times \frac{0.283\text{cubic meters}}{1.0\text{ cubic feet}} \times \frac{3600\text{ seconds}}{\text{hour}} \times 12.4\text{ hours/tidal cycle}$$

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After hydraulic simulation, water quality simulation can be conducted by introducing relevant reaction kinetics

2. 河川複雜水質模式的介紹和討論
Comprehensive River Water Quality Modeling

A. Modified Streeter-Phelps Equation (Reaction Kinetics)

Additional reaction kinetics are considered:

(1) Nitrification.

(2) Photosynthesis and respiration by aquatic plants.

(3) Benthal oxygen demand.

$$\frac{\mathrm{dD}}{\mathrm{d}\theta} = k_c L_c + k_n L_n - P_a + S_b - k_2 D$$

$$\text{At } \theta = 0, \mathrm{L_c} = \mathrm{L_{c0}}, \mathrm{L_n} = \mathrm{L_{n0}}, \mathrm{D} = \mathrm{D_0}$$

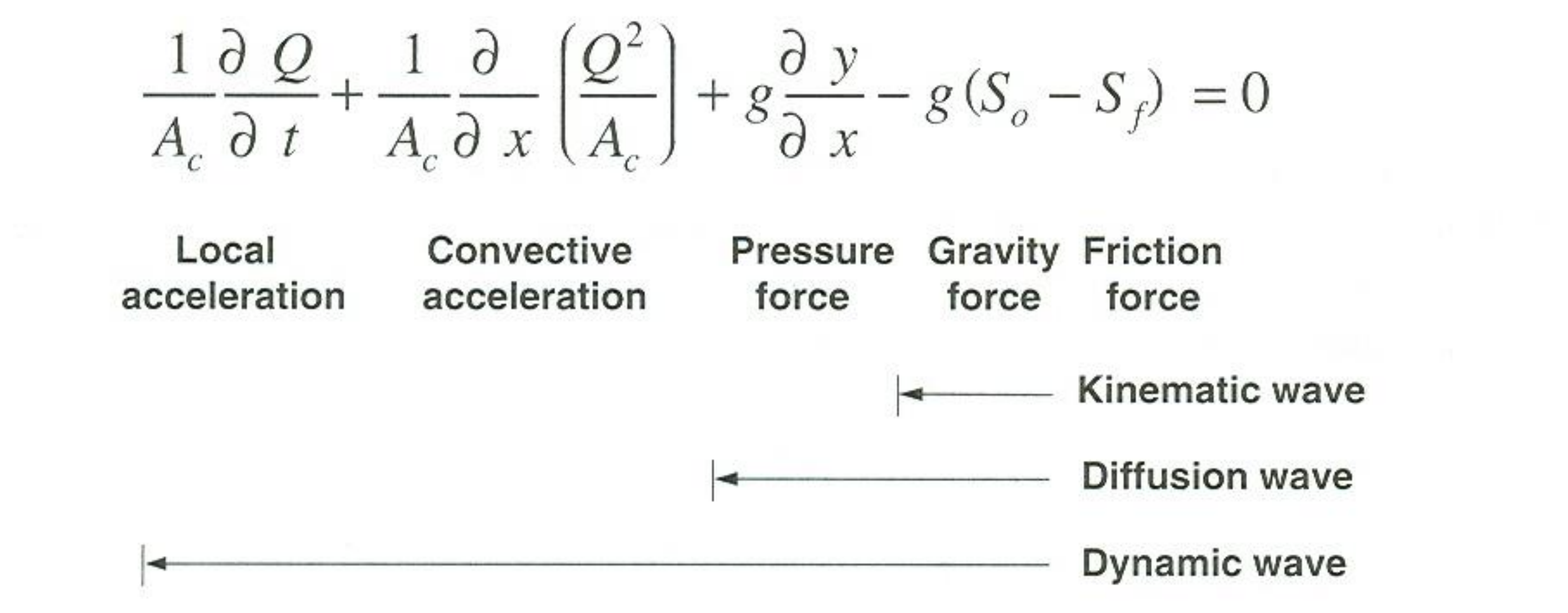
Solution

$$= \mathrm{D}(\theta) = \mathrm{D_0} e^{-\mathrm{k_2}\theta} + \frac{\mathrm{k_d L_c}}{\mathrm{k_2 - k_r}}[e^{-\mathrm{k_r}\theta} - e^{-\mathrm{k_2}\theta}]$$

$$+ \frac{\mathrm{k_n L_n}}{\mathrm{k_2 - k_n}}[e^{-\mathrm{k_n}\theta} - e^{-\mathrm{k_a}\theta}] - \frac{\mathrm{P_a}}{\mathrm{k_2}}(1 - e^{-\mathrm{k_2}\theta}) + \frac{\mathrm{S_b}}{\mathrm{k_2}}(1 - e^{-\mathrm{k_2}\theta})$$

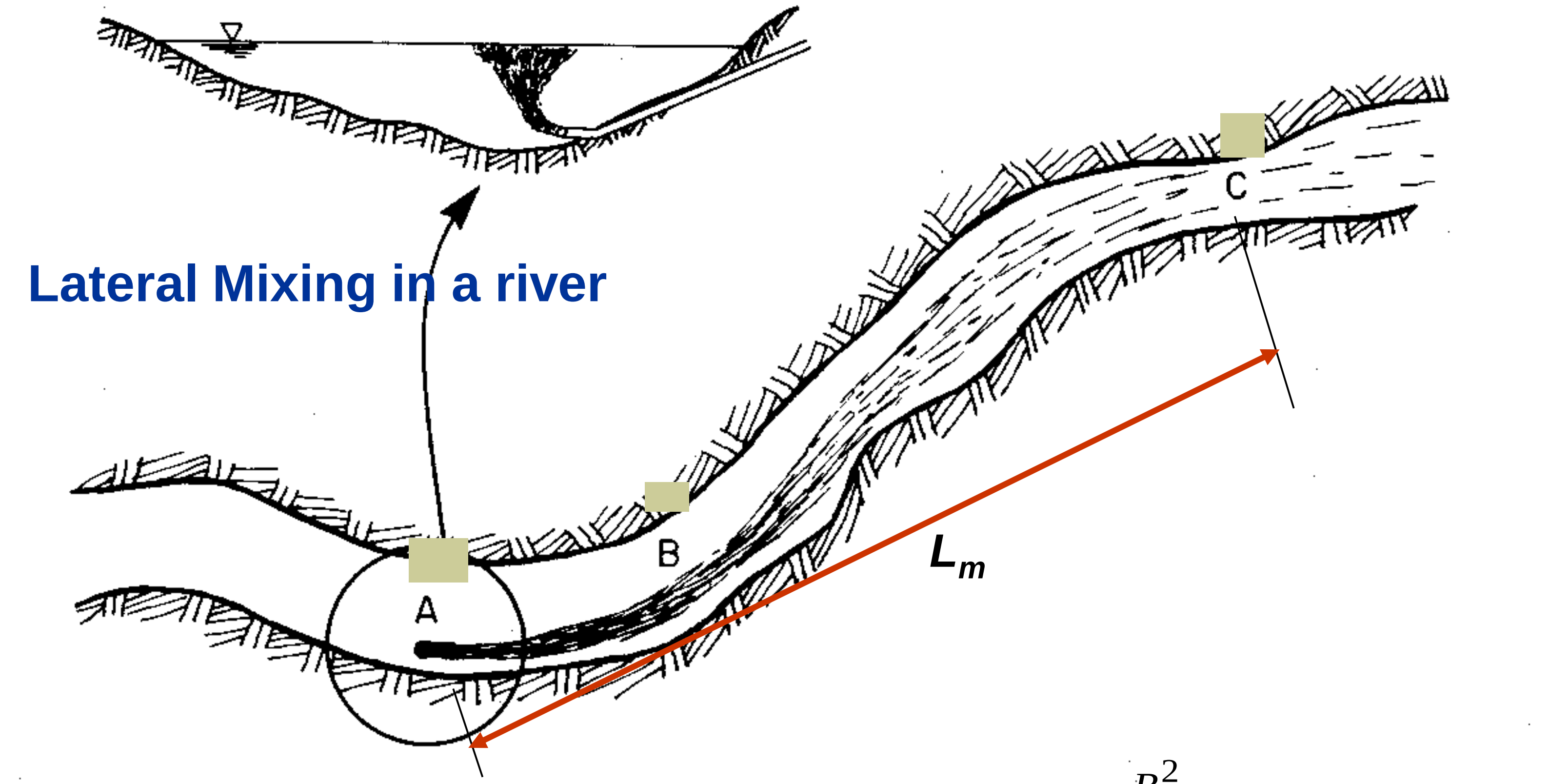
2. 河川複雜水質模式的介紹和討論
Comprehensive River Water Quality Modeling

B. Modified Streeter-Phelps Equation (Hydraulics)



$$\frac{1}{A_c}\frac{\partial Q}{\partial t}+\frac{1}{A_c}\frac{\partial}{\partial x}\left(\frac{Q^2}{A_c}\right)+g\frac{\partial y}{\partial x}-g\left(S_o-S_f\right)=0$$

Can we modifify the Streeter-Phelps Model by using a steady-state one-dimensional river models? (A discussion)



Lateral Mixing in a river

$$L_m = 0.4U\frac{B^2}{E_{lat}} \qquad (14.19)$$

Lateral dispersion coefficient, $E_{lat} = 0.6HU^*$

Shear velocity, $U^* = \sqrt{gHS}$

$S =$ Channel slope

A steady-state 1-D river model can be expressed as:

$$u\frac{dc}{dx} = E\frac{d^2c}{dx^2} - kc \qquad c = c_0\ as\ x = 0\ \ c \to 0\ as\ x \to \infty$$

The solution is

$$c = c_0 \exp\{-(\frac{kx}{u})[\frac{2}{\alpha}(\sqrt{\alpha+1}-1)]\}\ where\ \alpha = \frac{4Ek}{u^2}$$

For steady flow in a river, the distance required for lateral mixing (X_m) and for a decay of the pollutant to a factor of e^{-1}(X_d) are:

$$X_m = \frac{0.4UB^2}{E_{lat}}\ \ where\ E_{lat} = 0.6HU^*\ \ and,\ X_d = \frac{u}{k}$$

Note that the dispersion coefficient

$$\alpha = \frac{4Ek}{u^2} = \frac{4(0.011\frac{u^2B^2}{HU^*})k}{u^2} = \frac{0.024B^2k}{E_{lat}}$$

Therefore, for $X_d > X_m$, $\alpha < 0.06$

Findings: For the “decay distance” to exceed the “lateral mixing distance”, longitudinal dispersion must be negligible. Therefore, a river should either be simulated by a steady-state PFR or by a time-variable advection-dispersion model.

One-Dimensional Advection-Dispersion-Reaction River Model

Advection - diffusion - Reaction equation,

$$\frac{\partial \mathrm{c}}{\partial \mathrm{t}} = E\frac{\partial^2 c}{\partial x^2} - U\frac{\partial c}{\partial x} - \mathrm{kc}$$

Analytical solution can be derived by Laplace transform

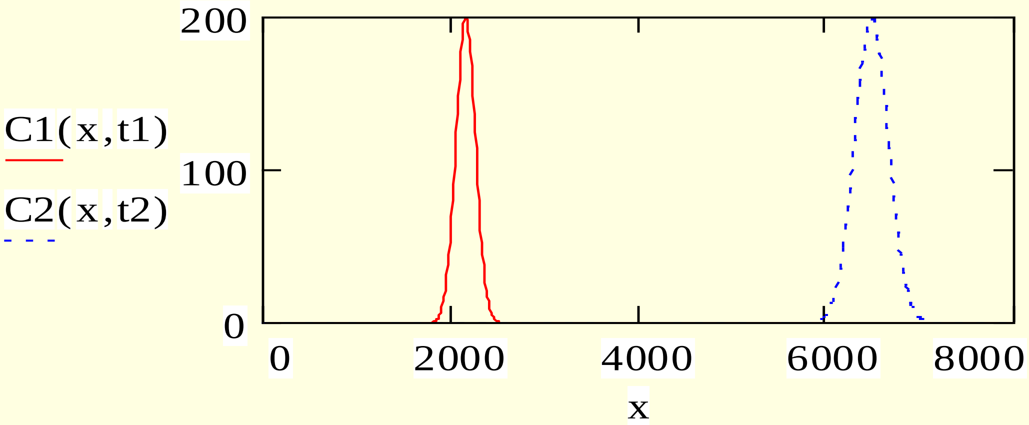
With a pulse input, the solution is

$$C(x,t) = \frac{m}{\sqrt{4E\pi t}}\exp[-\frac{(x-ut)^2}{4Et} - kt]$$

Example 10.3

$$k = 0, m = 500\,g/m^2; E = 0.1m^2/\mathrm{sec}; U = 0.2\,m/\mathrm{sec}$$

$$t1 = 3hrs; t2 = 9hrs$$



3. 污染物在河川的傳輸機制及數學模擬和模式係數值估算

Reaction Kinetics of Pollutants in Rivers

Deoxygentaion and Reaeration

Saturation concentration of dissolved oxygen, C_s

Henry’s law indicates the equilibrium concentration of a chemical in liquid and in the atmosphere across an atmosphere-liquid interface, and thus dictates the dissolved oxygen saturation in water

Henry’s law: $x = K P$

Where

x = mole fraction of the chemical in liquid phase

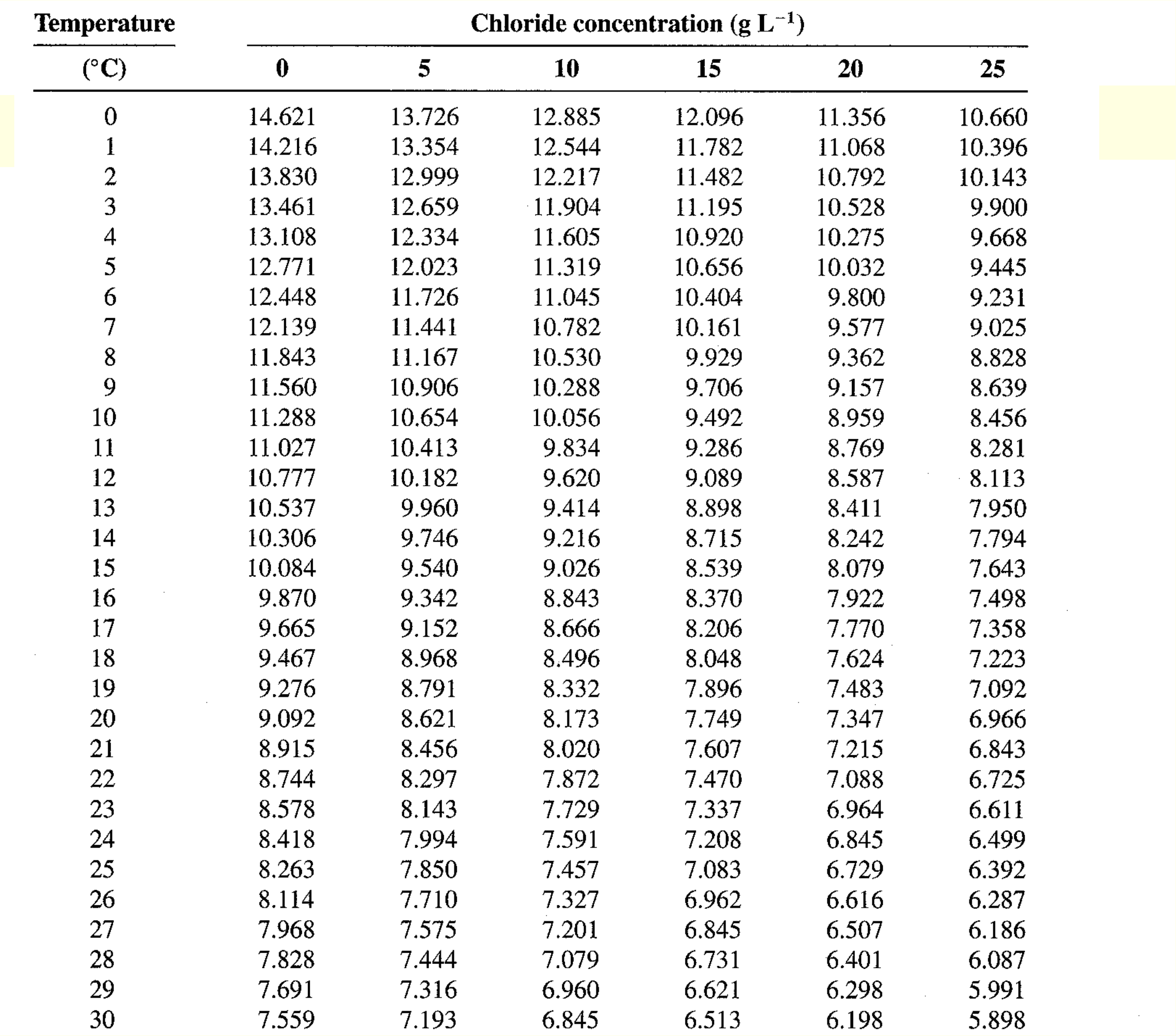
K = Henry’s law constant, atm^{-1}

P = partial pressure of the chemical in atmosphere, atm

Henry law constant for oxygen

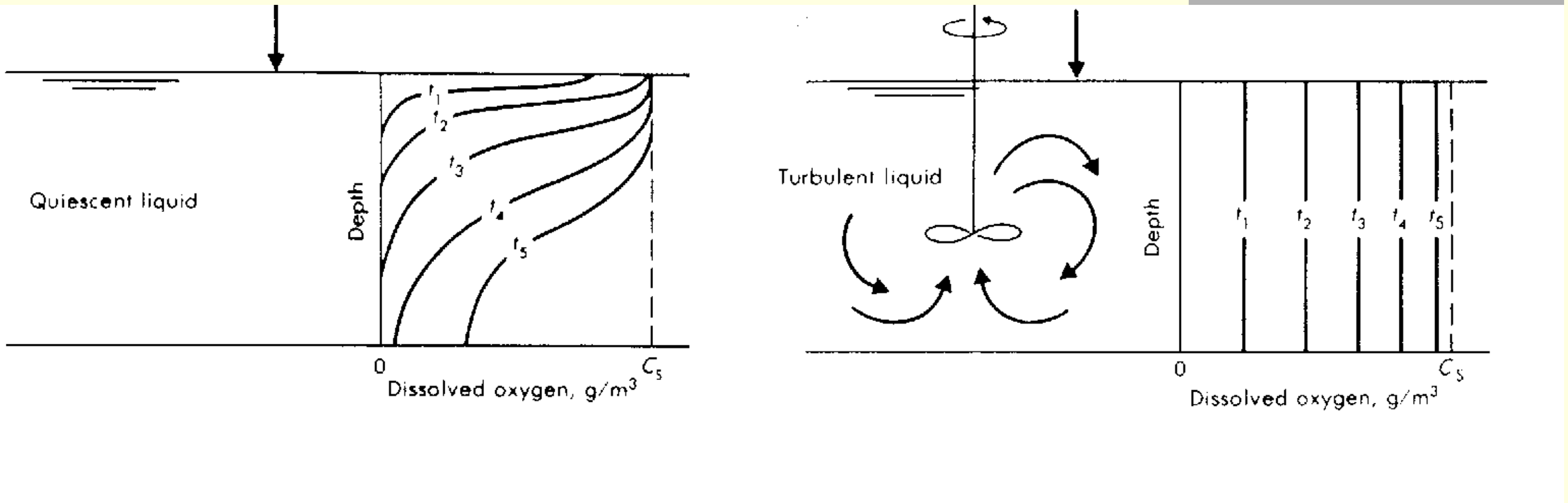
T, 0C	*K, atm^{-1}*
0	0.0000391
5	0.0000330
10	0.0000303
15	0.0000271
20	0.0000244
25	0.0000222
40	0.0000188
60	0.0000159

Dissolved Oxygen Saturation



Temperature (°C)	Chloride concentration (g L^{-1}) 0	5	10	15	20	25
0	14.621	13.726	12.885	12.096	11.356	10.660
1	14.216	13.354	12.544	11.782	11.068	10.396
2	13.830	12.999	12.217	11.482	10.792	10.143
3	13.461	12.659	11.904	11.195	10.528	9.900
4	13.108	12.334	11.605	10.920	10.275	9.668
5	12.771	12.023	11.319	10.656	10.032	9.445
6	12.448	11.726	11.045	10.404	9.800	9.231
7	12.139	11.441	10.782	10.161	9.577	9.025
8	11.843	11.167	10.530	9.929	9.362	8.828
9	11.560	10.906	10.288	9.706	9.157	8.639
10	11.288	10.654	10.056	9.492	8.959	8.456
11	11.027	10.413	9.834	9.286	8.769	8.281
12	10.777	10.182	9.620	9.089	8.587	8.113
13	10.537	9.960	9.414	8.898	8.411	7.950
14	10.306	9.746	9.216	8.715	8.242	7.794
15	10.084	9.540	9.026	8.539	8.079	7.643
16	9.870	9.342	8.843	8.370	7.922	7.498
17	9.665	9.152	8.666	8.206	7.770	7.358
18	9.467	8.968	8.496	8.048	7.624	7.223
19	9.276	8.791	8.332	7.896	7.483	7.092
20	9.092	8.621	8.173	7.749	7.347	6.966
21	8.915	8.456	8.020	7.607	7.215	6.843
22	8.744	8.297	7.872	7.470	7.088	6.725
23	8.578	8.143	7.729	7.337	6.964	6.611
24	8.418	7.994	7.591	7.208	6.845	6.499
25	8.263	7.850	7.457	7.083	6.729	6.392
26	8.114	7.710	7.327	6.962	6.616	6.287
27	7.968	7.575	7.201	6.845	6.507	6.186
28	7.828	7.444	7.079	6.731	6.401	6.087
29	7.691	7.316	6.960	6.621	6.298	5.991
30	7.559	7.193	6.845	6.513	6.198	5.898

Reaeration kinetics



The rate of reaeration depend on stream’s dissolved oxygen deficit and turbulence. One of the predictive equation, O’Connor and Dobbins

Equation is:

$$k_2 = 12.9 \frac{U^{1/2}}{H^{3/2}}$$

where

k_2 = reaeration coefficient (base e) per day
U = velocity of flow, ft/sec
H = depth of flow, ft

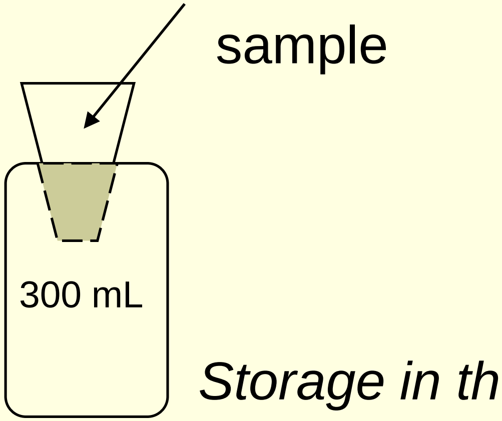
Reaeration kinetics

Reaeration coefficient estimated by using a predictive equation is not reliable. If possible, the reaeration coefficient should be determined by field experiments.

Reference:

Liu, C.C.K. and Fok, Y.S. (1983). Stream Waste Assimilative Capacity Analysis Using Reaeration Coefficients Measured by Tracer Techniques. ***Water Resources Bulletin***, *Journal of the American Association of Water Resources (AWRA),* Vol.19, No.3, pp.439-445.

Measuring Concentration of Organic Wastes (Biochemical Oxygen Demand)



the amount of oxygen consumed during microbial utilization of organics is call the biochemical oxygen demand (BOD).

Storage in the dark at 20 ^{0}C

$$y(t) = \frac{DO_i - DO_t}{P}$$

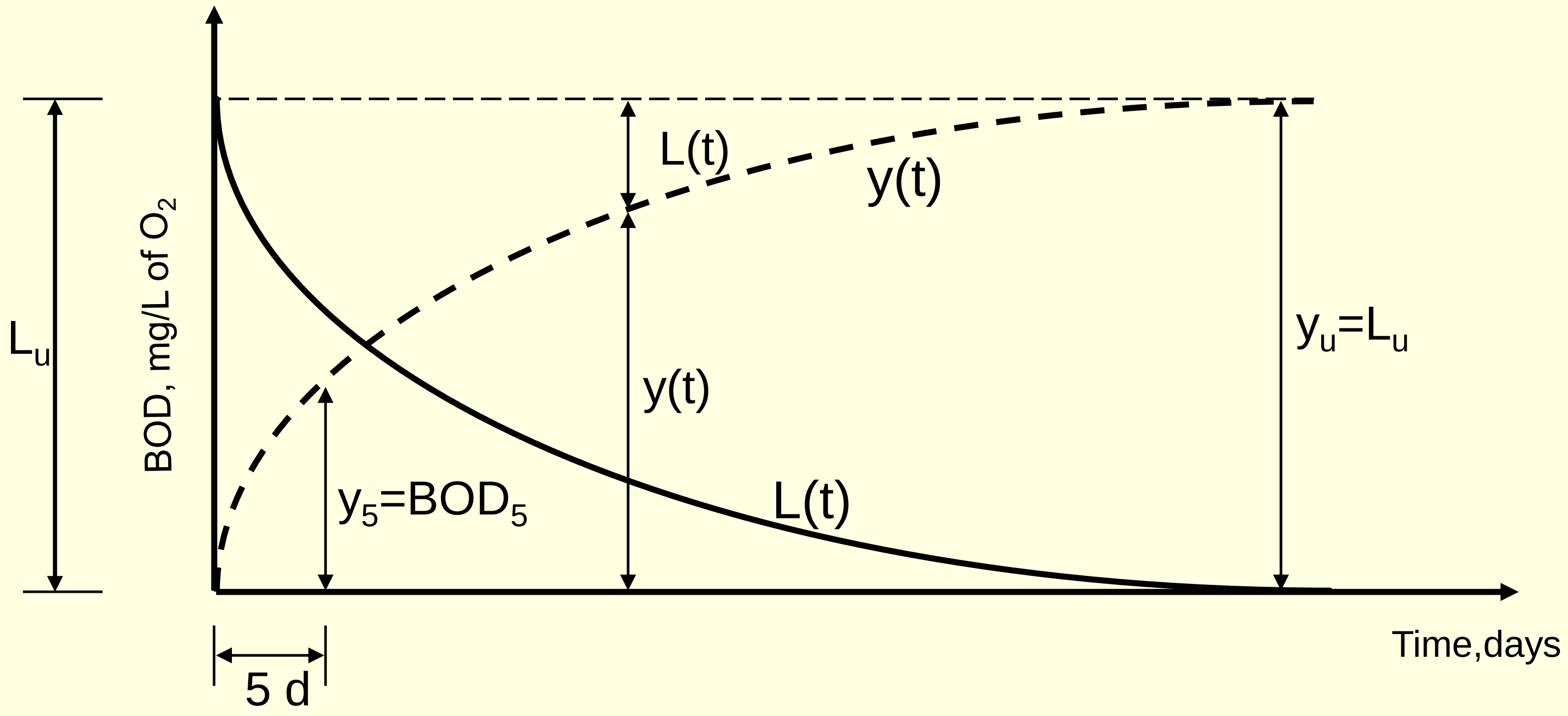
Where

Y(t) is the BOD consumed after a time of t days.

DO_i and DO_t are initial and t-day dissolved-oxygen concentrations (mg/L)

P the decimal fraction of the sample in the 300-ml bottle.

BOD Consumed and BOD Remaining



y(t)=BOD ***consumed***, mg/L

L(t)=BOD ***remaining***,mg/L

L_u= ultimate (carbonaceous)BOD,mg/L

Deoxygenation Kinetics

BOD kinetics

$$\frac{dL}{dt} = -k_1 L$$

$$L(t) = L_u \exp(-k_1 t)$$

Where
k_1 = Laboratory deoxygenation coefficient, d-1
L (t) = BOD remaining, mg/L (a time variable)
L_0 = Ultimate BOD, mg/L (a constant with time)

BOD consumed, y(t)

$$y(t) = L_u - L(t)$$

$$= L_u[1 - \exp(-k_1 t)]$$

Where
y(t) = BOD consumed, mg/L (a time variable)

Determination of in-stream Deoxygenating Coefficient

1. Computation based on stream survey data.

2. Use empirical formula

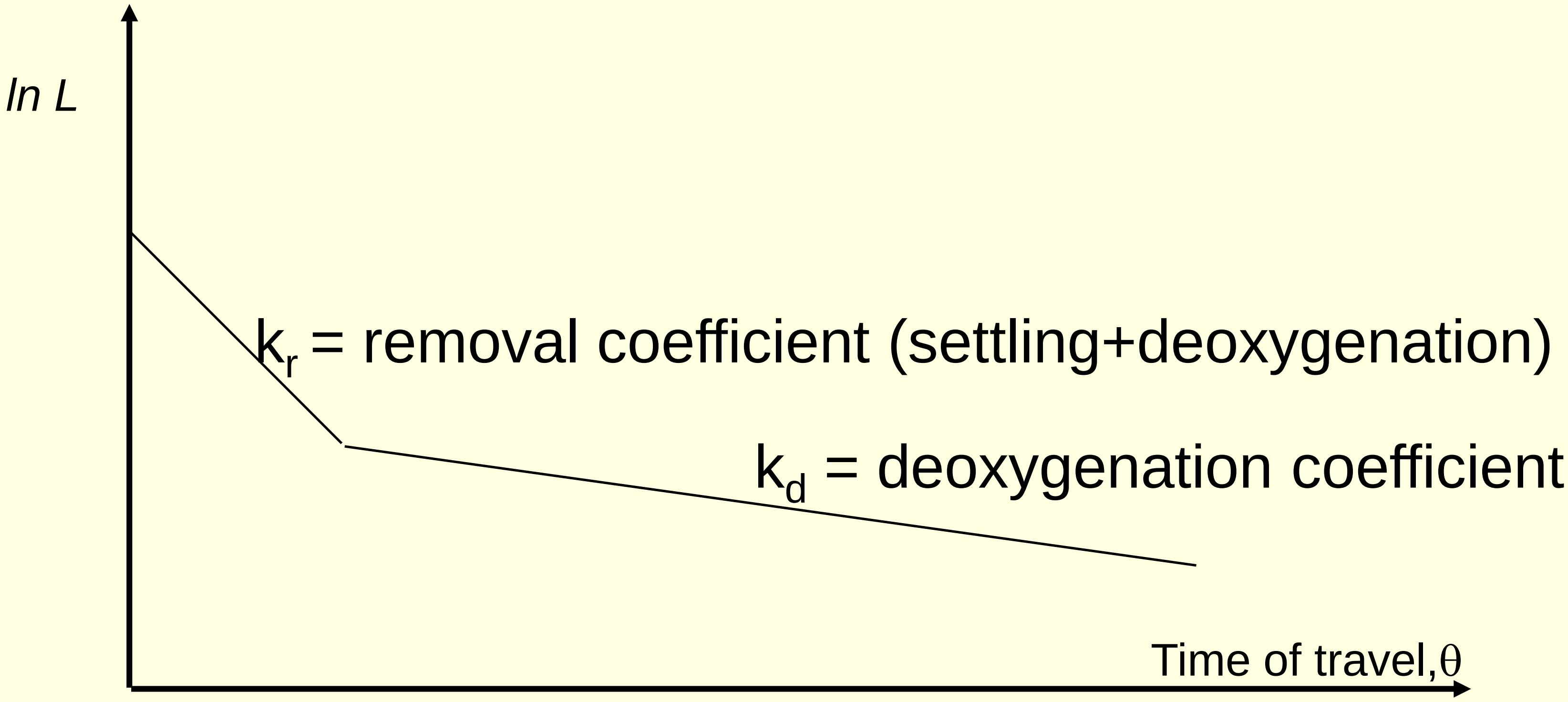
(*Ref.US EPA Research Rep."Rates,Constants, and Kinetics Formulations in Surface Water Quality Modeling, EPA-600/3-78-105, 1978*)

$$k_d = k_1 + n(V/D)$$

where

k = in-stream deoxygenation coefficient, per day
V = Stream velocity, ft/sec
D = Stream depth, ft
n = coefficient of bed activity

Kinetics of In-stream BOD deoxygenation and removal



k_r = removal coefficient (settling+deoxygenation)

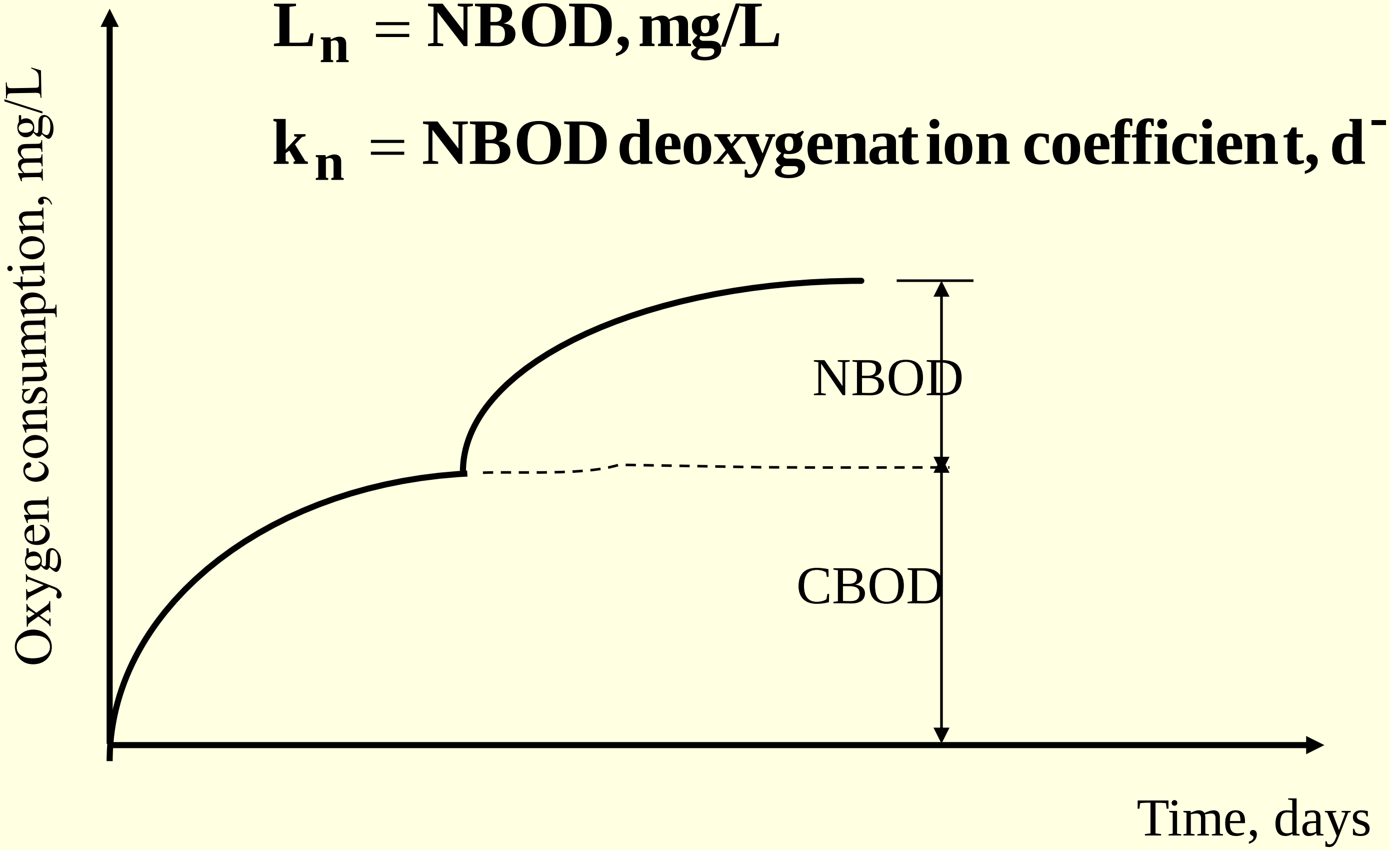
k_d = deoxygenation coefficient

Nitrification and the Second stage BOD

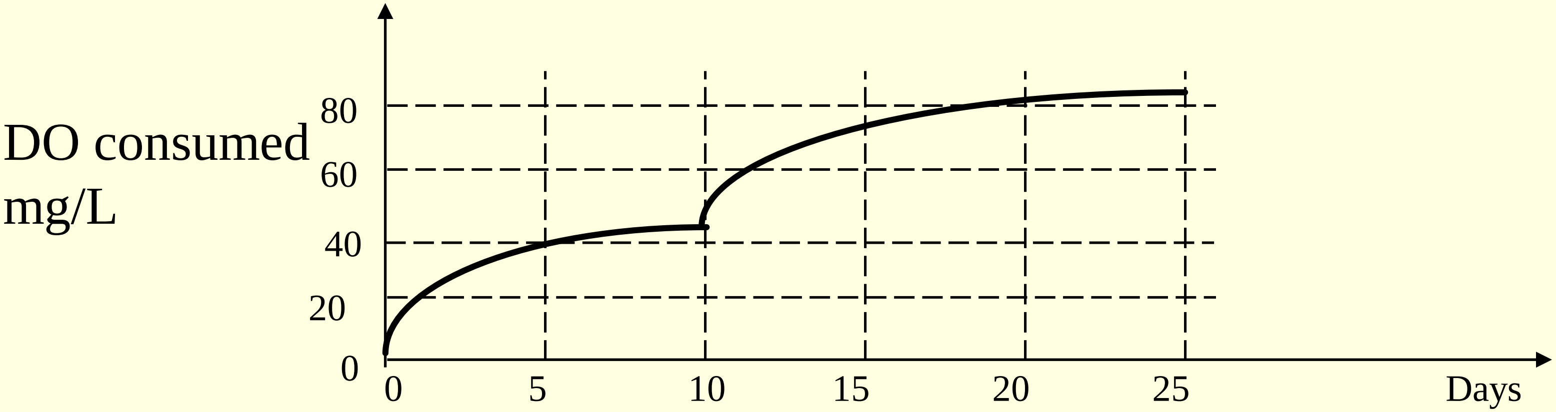
$$\textbf{Kinetic Equation :} \quad \frac{dL_n}{dt} = -k_n L_n$$

$$L_n = \text{NBOD, mg/L}$$

$$k_n = \text{NBOD deoxygenation coefficient, } d^{-1}$$



Example A long term BOD test was conducted of a wastewater sample at a laboratory. The data of this test are plotted in a diagram below.



Determine:

(1) What is the BOD_5 of this wastewater?

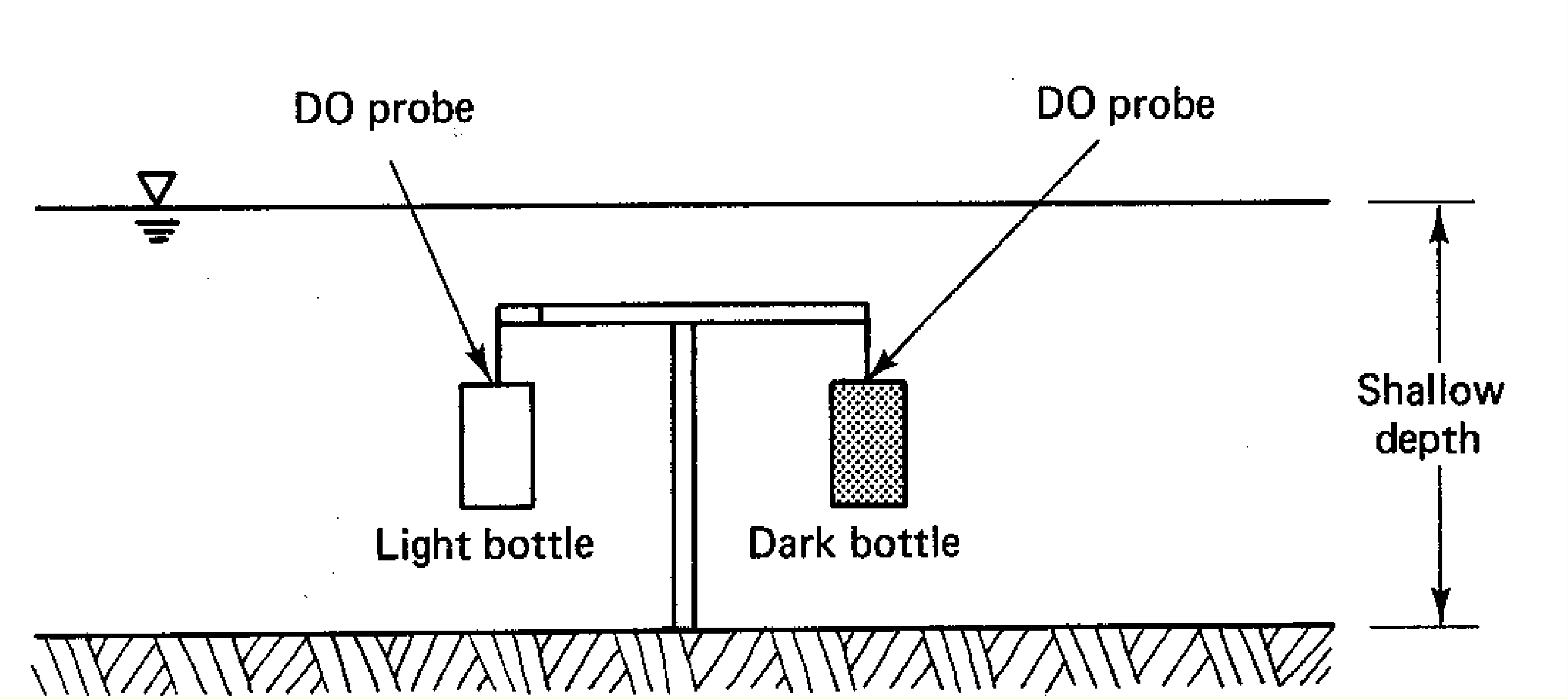
(2) What is the CBOD of this wastewater?

(3) What is the NBOD of this wastewater?

(4) What is the CBOD deoxygenation rate constant, k_d of this wastewater?

Photosynthesis and Respiration

Light and dark bottles and chambers for measurement of photosynthesis and respiration



Diurnal DO Variation in a Biologically Active Stream

In a stream containing phytoplankton biomass and benthic plants, its DO content is affected by the processes of photosynthesis and respiration. Photosynthesis is the biological synthesis of organic compounds by chlorophyll bearing plants in the presence of solar energy. A by-product of this process is oxygen. On the other hand, oxygen is consumed by living organisms as a process of their respiration. Therefore, for a biologically active stream, observed DO content is the results of several dynamic processes including photosynthesis and respiration.

Ideally, a natural water body with significant biological oxygen production and consumption is analyzed in terms of a time varying model which makes stream DO content a function of both time and space. However, the application of a time varying model in many water quality management studies is constrained for a lack of field data and due to numerical complexities in its solution. Therefore, a steady state model is still the most popular tool in water quality analysis.

A set of equations (Liu, 2005) which separate time varying effects of photosynthesis/respiration from observed DO were developed. The DO profile thus modified constitutes a sound basis for the calibration of a steady- state stream water quality model for a biologically active stream.

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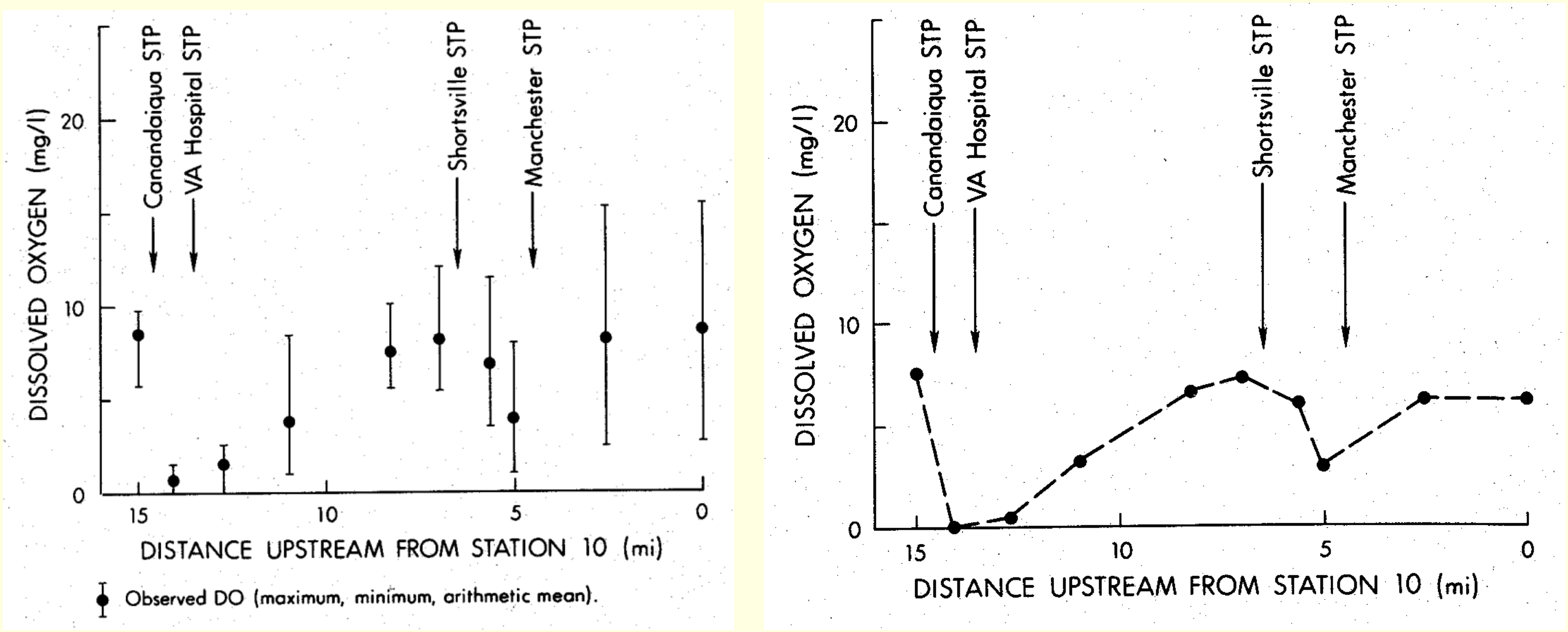

(a) Observed DO in a biologically active stream

(b) Estimated Steady State DO Profile

DO variation in Canandaiqua Outlet in Central Yew York, July 18-19, 1978.

Sediment Oxygen Demand (Benthic Demand)

Ala Wai Canal in Honolulu, Hawaii, where benthic demand is a major dissolved oxygen sink