Mathematical Modelling of Pollutants Transport in Surface Waters

Ph. D. Course

(15 weeks/ 2 hours per week)

By

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Surface Water

Surface water is any water that collects on the surface of the earth. This includes oceans, seas, estuaries, lagoons, rivers, lakes or wetlands. The first four water bodies are called tidal water bodies, in which tides occur. Tides are periodic rise (flood) and fall (ebb) of the water in rhythmic daily pattern. Gravity is one major force that creates tides. Newton explained that ocean tides result from the gravitational attraction of the sun and moon on the oceans of the earth. High tides and low tides are caused by the moon. The moon's gravitational pull generates something called the tidal force. The tidal force causes Earth—and its water—to bulge out on the side closest to the moon and the side farthest from the moon. These bulges of water are high tides.

Classification of Tides

Tides are frequently classified according to the diurnal inequality they display. They are classified into four groups as follows:

- Semidiurnal (SD): two nearly equal high waters (HWs) and two nearly equal low waters (LWs) approximately uniformly spaced over each lunar day.
- Mixed, mainly semidiurnal (MSD): two HWs and two LWs each lunar day, but with marked inequalities in height and irregularities in spacing.
- Mixed, mainly diurnal (MD): sometimes two unequal HWs and LWs at irregular spacing over a lunar day, and sometimes only one HW and one LW in a day.
- Diurnal (D): only one HW and one LW each lunar day.

Water Quality Problem Identification

From the point of view of water quality control and management, it is desirable to examine water quality problems in terms of specific constituents or groups of constituents which are discharged as a result of man's activities and natural phenomena. Table **1** presents a list which relates constituents to water quality. One of the initial steps in the planning effort with respect to water quality modeling, is the identification of the water quality problems presently observed and those projected under future conditions of population growth and development. Having identified the significant present and future water quality problems, it is then necessary to select the constituents which are discharged to the environment, from natural and manmade activities, that are responsible for water quality problems.

Table 1
Some waste discharge constituents and related water quality problems

Waste discharge constituent	**Water Quality and water use problem**
Total dissolved solids (TDS)	Agricultural, industrial and domestic water supply
Temperature	Dissolved oxygen, aquatic balance
Carbonaceous BOD	Dissolved oxygen - Nutrient
Organic Nitrogen (Organic -N)	Dissolved oxygen - Nutrient
Ammonium	Dissolved oxygen - Nutrient
Nitrite (NO_2) and Nitrate (NO_3)	Nutrient - Dissolved oxygen - water supply
Phosphate	Nutrient
Toxic metals and inorganics	Water supply - food chain
Toxic organics	Water supply – recreational usage
Bacteria	Water supply – recreational usage
Virus	Water supply – recreational usage
Floating substances	Recreational usage
Suspended Solids	Recreational usage – dissolved oxygen - nutrient – light limitations
Radioactive substances	Water supply

Mathematical Modelling of Surface Water Pollution

Water quality models are used to predict the concentration of any constituent (or contaminant) in water as a function of time and position (x, y and z). These models are classified based on number of spatial dimensions into;

1. Zero order model.
2. One dimensional model.
3. Two dimensional model in plan view.
4. Two dimensional model in side elevation.
5. Three dimensional model

All of above models are derived based on conservation of mass equation.

Conservation of Mass Equation

Conservation of mass equation for the temporal and three dimensional spatial variations of any constituent concentration in water is written as;

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(D_X\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)+S_T$$

Where;

C= constituent concentration, mg/l.

u, v and w = velocity components in x-, y- and z-directions, respectively.

D_x, D_y and D_z are diffusion coefficients in x-, y- and z-directions, respectively.

S_T= Sink/ Source terms.

Diffusion

Diffusion is an important process that results in mass mixing. Diffusion is mass transport in response to a concentration gradient. Thus contaminants present in *water will diffuse away from the plume in all directions in response to concentration gradients.*

Zero Dimensional Model

The main purpose of a zero dimensional model is to estimate the seriousness of a waste discharge problem. In this model, the tide period is the smallest reasonable unit of time. Therefore, zero order models predict a concentration field of the form;

$$\bar{C} = f(\bar{t}\,) \qquad \ldots (2)$$

Where $\bar{t}$ is the time considered to vary in increments equal to a tidal period. zero dimensional models cannot reproduce the dynamic aspect of the tide motion.

Integrating Eq.1 over the volume of a tidal water body such as an estuary results in;

$$\frac{d\bar{C}}{d\bar{t}} + \frac{\bar{C}\bar{F}}{\bar{V}} = \frac{\overline{C_0}\bar{R}}{\bar{V}} + \frac{\overline{C_w Q_w}}{\bar{V}} + \bar{S}_T \qquad \ldots (3)$$

where; $\bar{C}$ is the average concentration of the considered constituent, $\bar{F}$ the net volume of water lost from the estuary during each tide cycle, $\bar{C}_0$ is constituent concentration in the river inflow, $\bar{R}$ is the volume of river inflow, $\bar{Q}_w$ is the waste discharged into the estuary and $\bar{C}_w$ is constituent concentration in the wastewater and $\bar{V}$ is the average water volume in the estuary. Although $\bar{C}$, $\bar{F}$, $\bar{R}$, $\bar{Q}_w$, $\bar{C}_w$ and $\bar{S}_T$ are averaged over a tidal period, they are all function of $\bar{t}$.

Assuming $\bar{F}$ is proportional to the volume of the tidal prism, $\bar{P}$, which is the volume of water in an estuary between mean high tide and mean low tide, or the volume of water leaving an estuary at ebb tide. $\bar{P}$ is obtained as;

$$\bar{P} = H\,A \qquad \ldots (4)$$

where H is the average tidal range and A is the average surface area of the basin.

One Dimensional Model

One dimensional model can give accurate description of waste concentration and movement in a long well mixed estuary. It may indicate the form of concentration distribution and enable different waste management proposals to be compared. The predicted concentration field has the form;

$$C = f(x,t) \qquad \ldots(5)$$

The one dimensional transport equation can be obtained by integrating Eq.1 over the flow cross sectional area and it can be written as;

$$\frac{\partial AC}{\partial t} + \frac{\partial (AV_x C)}{\partial x} = \frac{\partial}{\partial x}\left(AK_X \frac{\partial C}{\partial x} \right) + S_T \qquad \ldots(6)$$

Where x is longitudinal direction, V_x is flow velocity in x- direction, A is cross sectional area of flow and K_x is dispersion coefficient in x- direction.

Two Dimensional Models- Plan View

A two dimensional plan view model allows concentration variations in longitudinal and lateral directions. It is suitable for vertically well mixed shallow water bodies. It predicts a concentration field of the form;

$$C = f(x,y,t) \qquad \ldots(7)$$

A two dimensional plan view model is based on the vertically integrated conservation of mass equation;

$$\frac{\partial (HC)}{\partial t} + \frac{\partial (HUC)}{\partial x} + \frac{\partial (HVC)}{\partial y} = \frac{\partial}{\partial x}\left(HK_X \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y}\left(HK_y \frac{\partial C}{\partial y} \right) + S_T \qquad \ldots\mathbf{(8)}$$

Where;

C= depth averaged constituent concentration, mg/l.

U and V= depth averaged flow velocity components in x- and y- directions, respectively, m/sec.

K_x and K_y= dispersion coefficients in x- and y- directions, respectively, m^2/sec.

H= total water depth in the stream, m, which is a function of x and y.

Two dimensional plan view models represent lateral and longitudinal lateral variations in velocity and constituents concentration which arise in all real estuaries and bays because of non-uniformity of cross sections, branching channels and bends. However, these models are restricted to vertically well mixed estuaries, and the effects of vertical density gradients are not represented satisfactory.

Shallow Water Body

The water body is said to be shallow if its width to depth ratio is greater than ten.

Dispersion

Dispersion refers generally to phenomena that cause fluid mixing. Dispersion is more accurately described as the apparent mixing due to unresolved advective movement at scales finer than captured by the mean advection model.

Depth averaged value definition

Consider an estuary with a cross sectional area of flow shown in Fig.1. this figure shows that the estuary has arbitrary bathymetry, *b*. Thus, the distance from mean sea level to the bottom of the estuary is a function of *x* and *y*. Moreover, due to the tidal motion, the surface elevation from mean sea level h is a function of time as well as *x* and *y*. The total distance from the bottom of the estuary to the surface is denoted by *H* and is equal to b + *h*.

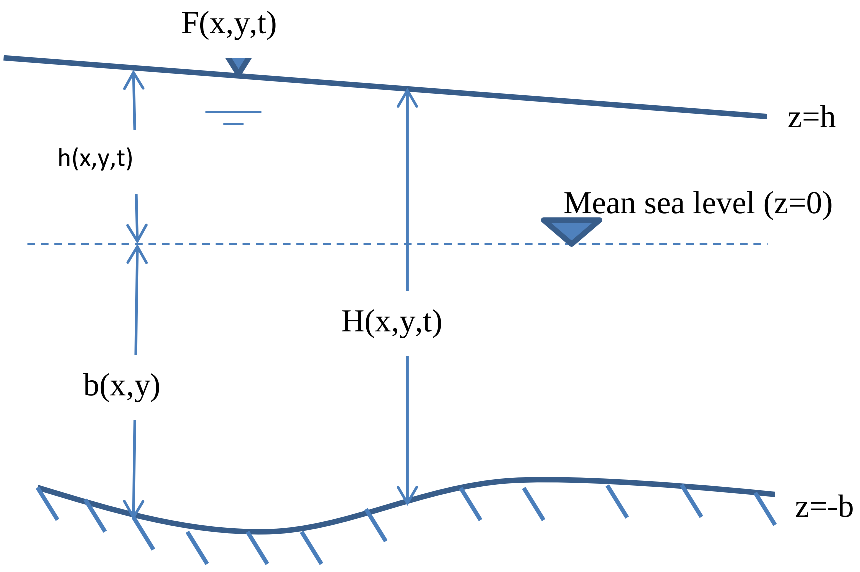


Fig.1: Cross section of a typical estuary

Assume q is any dependent variable, then, the depth averaged value of q (denoted by Q) is obtained as;

$$Q = \frac{\int_{-b}^{h} q dz}{H} \qquad \ldots(9)$$

Where;

b = bottom level.

h= water surface level.

H=total water depth.

Two Dimensional Models- Side Elevation

In density stratified estuaries, the transverse variation in constituent concentration may be much smaller than the longitudinal and vertical variations. Under these circumstances, two dimensional side elevation models are used. These models predict constituent concentration field of the form;

$$C = f(x, z, t) \qquad \ldots(10)$$

For these models, the transport equation is developed by integrating Eq.1 over the width of the estuary (laterally integrated mass transport equation);

$$\frac{\partial(BC)}{\partial t}+\frac{\partial(BUC)}{\partial x}+\frac{\partial(BWC)}{\partial z}=\frac{\partial}{\partial x}\left(BK_X\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(BK_Z\frac{\partial C}{\partial z}\right)+S_T \quad \textbf{...(11)}$$

Where;

C= width averaged constituent concentration, mg/l.

U and W= width averaged flow velocity components in x- and z- directions, respectively, m/sec.

K_x and K_z= dispersion coefficients in x- and z- directions, respectively, m^2/sec.

B= stream width witch is a function of x and z.

Two dimensional side elevation models are limited to narrow estuaries that are well mixed laterally.

Three Dimensional Models

Three dimensional models allow the complete spatial distribution of the constituent concentration field to be predicted. Herein;

$$C=f(x,y,z,t) \qquad ...(12)$$

Hint; Eq.1 represents the three dimensional transport of any constituent.

Source/ Sink Term

The source/sink term (S_T) can be expressed as;

$$S_T=R+L \qquad ...(13)$$

Where;

R= time rate of increase or decrease of constituent concentration $(\frac{dc}{dt})$ due to various transformations or reaction processes.

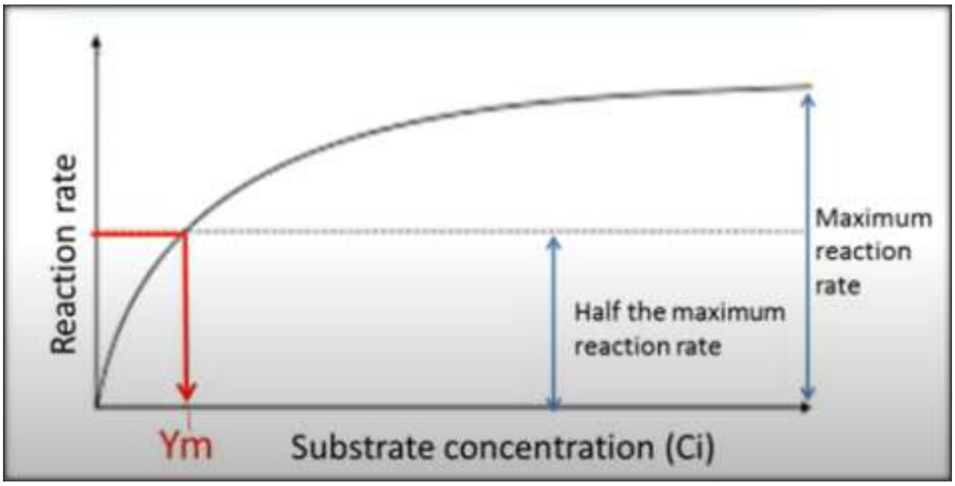
L= time rate of constituent concentration variation due to external waste source.

Transformations affecting the increase or decrease of constituent concentration are often expressed in first order kinetic terms. Thus it is assumed that transformation rates are proportional to constituent concentration. However, some of transformation rates are related to constituent concentration through Michael's-Menton reaction kinetics. Eqs. (14) and (15) describe the first order and Michael's-Menton reaction kinetics, respectively;

$$\frac{dC_i}{dt} = K_i C_i \qquad \ldots(14)$$

$$\frac{dC_i}{dt} = K_{ik} \frac{C_i\ C_k}{Y_m + C_i} \qquad \ldots(15)$$

Where; K_i= Reaction (decay or production) rate ($time^{-1}$), K_{ik} = rate of transformation from the i-constituent to the k-constituent ($time^{-1}$), and Y_m= half saturation constituent concentration.



Representation of reaction term (R)

Water constituents may be conservative or non- conservative constituents. The conservative constituents are those that their concentrations hardly change over time or that change very slowly (non-reactive constituents). On the other hand, non-conservative constituents are subjected to transformation processes like biological reactions. In this course, the considered water constituents include;

(1) salinity, (2) organic-N, (3) ammonium-N, (4) nitrite-N, (5) nitrate-N, (6) carbonaceous BOD, (7) volatile organic matter, (8) dissolved oxygen, (9) chlorophyll "a", (10) crude oil, (11) heavy metals and (12) Phosphate-P. C_1, C_2, C_3, C_4,….and C_{12} will denote the concentration of each of salinity, organic-N,….and phosphate, respectively.

According to each of above constituents, the transformation processes, their rate coefficient, and subsequently the formulation of the reaction term (R_i) can be given as follows:

1. Salinity (C_1):

Salinity is a conservative constituent. Thus; $R_1 = 0.0$

2. Organic-N (C_2):

In natural streams, organic-N transforms to ammonium-N by hydrolysis process;

$$\text{Org-N} \xrightarrow{H_2O} \text{NH}_4\text{-N} \quad \text{... (16)}$$

The reaction term, R_2, can be expressed as;

$$R_2 = -K_2 C_2 \quad \text{…(17)}$$

Where; K_2 = hydrolysis coefficient (day-1). This coefficient can be obtained as;

$$K_2 = 0.088\,(1.05)^T \quad \text{…(18)}$$

where; T is the temperature (°C).

3. **Ammonium-N (C_3)**

The kinetic and transformation processes that affect the concentration of ammonium-N are; (1) exsolution of ammonium-N to atmosphere, (2) biological oxidation of ammonium-N to nitrite-N by Nitrosomonas bacteria, and (3) production of ammonium-N by hydrolysis of organic-N. Thus, the reaction term R_3 can be expressed as;

$$R_3 = -K_e C_3 - K_3 C_3 + K_2 C_2 \quad \ldots(19)$$

in which; K_e= exsolution coefficient (day^{-1}) and K_3= rate coefficient of ammonium-N oxidation (day^{-1}). The first term ($-K_e C_3$) on the right hand side represents loose of ammonium-N by exsolution which depends on environmental factors including pH, Temperature, surface turbulent, and wind velocity. K_e can be determined as;

$$\mathrm{K}_e = 0.01(1 - \mathrm{Fa}) + 0.5\mathrm{Fa} \quad \ldots(20)$$

The undissociated fraction of ammonium-N (Fa) is a function of both pH and temperature;

$$F_a = \frac{10^{pH}}{\frac{K_b}{K_w}+10^{pH}} \quad \ldots(21)$$

where; K_b = Ionization constant of aqueous ammonium-N and K_w = ionization constant of water. Mathematically, the ratio K_b/K_w can be expressed in terms of temperature as;

$$K_b/K_w = -3.398\mathrm{Ln}\,(0.0241T\times 10^9) \quad \ldots(22)$$

The second term on right hand side of Eq.20 represents loss of ammonium-N by biological oxidation. The rate coefficient of ammonium oxidation (K_3) can be calculated either of Eq.24 or Eq.25 as;

$$K_3 = 0.833T + 0.0646x_o + \frac{2.1234}{U_T} \quad \ldots(23)$$

$$K_3 = 0.073(1.017)^T \quad \ldots(24)$$

Where; T= temperature (°C) , x_o= density of Nitrosomonas bacteria, U_T= total flow velocity (m/sec) and K_3 is the rate of ammonium-N oxidation (day^{-1}). It is important to mention here that involvement of biological oxidation process depends on the presence of Nitrosomonas bacteria in water.

The third term of Eq.20 represents the production of ammonium-N by hydrolysis of organic-N. Herein the rate of organic-N decay is equal to ammonium-N production assuming there is no loss or gain of nitrogen in the transformation from organic-N to ammonium-N.

4. Nitrite-N (C_4)

The main processes affecting the concentration of nitrite-N are; (1) biological oxidation of nitrite-n to nitrate-N by Nitrobacter bacteria, (2) production of nitrite-N from ammonium-N by biological oxidation. Thus the reaction term, R_4, can be expressed as;

$$R_4 = -K_4 C_4 + K_3 C_3 \qquad \dots(25)$$

where; K_4= rate coefficient of biological oxidation of nitrite-N. At 20°C, K4 is equal to 0.25/day. While, at any other temperature, K_4, can be obtained as;

$$K_{4(T°C)} = K_{4(20°C)} \times 1.0826^{T-20} \qquad \dots(26)$$

4. Nitrate-N (C_5)

Nitrate-N is produced by biological oxidation of nitrite-N, at the same time it is assimilated by aquatic plants (phytoplankton). The reaction term R_5 can be expressed as;

$$R_5 = -K_{5P} \frac{C_5 * C_{ph}}{Y_m + C_5} + K_4 C_4 \qquad \dots(27)$$

Where; K_{5P} =1/day (light hours); 0.05/day (dark hours).

C_{ph}= concentration of phytoplankton-N.

Or, R5 can be expressed using first order kinetic for the decay process as;

$$R_5 = -K_5 C_5 + K_4 C_4 \qquad \dots(28)$$

Where; K_5=0.001/day

There are other reaction processes which affect the concentration of the four states of elemental nitrogen considered above. These processes include:

1- Ammonium-N uptake by and assimilation by phytoplankton.

2- Fixing of atmospheric nitrogen.
3- Denitrification of nitrate-N.
4- Zooplankton grazing on phytoplankton.
5- Lysis and leakage of organic-N through cell walls.
6- Ammonium- N regeneration by living cells.
7- Settling of organic-N.
8- Natural death of microorganisms.

If these processes are to be considered, then, the model must simulate the distribution of other states of elemental nitrogen like;

- Phytoplankton- N.
- Zooplankton- N.
- Particulate organic- N.

6. Carbonaceous Biochemical Oxygen Demand (C_6)

The direct discharge of wastewater containing organic matter into streams can have destructive effects on stream water quality by creating a high oxygen demand on the receiving water. Microorganisms present in the stream and wastewater will slowly oxidize the introduced organic waste, and in doing so, will consume the available oxygen normally present in the stream. Under these conditions, the oxygen levels cannot be replaced by re-aeration at a quick enough rate for larger organisms (such as fish) to survive.

Carbonaceous Biochemical Oxygen Demand (CBOD) is a single stage reaction defining the quantity of dissolved oxygen used by organisms in the water column as they consume the organic materials. It is an indication of organic content in water. The rate of CBOD decay, R_6, can be expressed as;

$$R_6 = -K_C C_6 \qquad \ldots(29)$$

Where K_c = CBOD decay coefficient (day^{-1}). The value of K_c for wastewater and surface water can be determined by laboratory analysis. This involves a series of CBOD determinations made over time and applying analytical or graphical methods for evaluating the laboratory results. These methods include (1) Thomas graphical method, (2) Method of moment and (3) Log difference method. We will consider Thomas graphical method for K_c determination.

The dependency of K_c on temperature can be given as;

$$K_{c(T°C)} = K_{c(20°C)} \times 1.047^{T-20} \qquad \ldots(30)$$

Thomas Method

This method is a graphical procedure based on the following function;

$$\left(\frac{t}{y}\right)^{1/3} = (KL)^{-1/3} + \frac{K^{2/3}}{6L^{1/3}}t \qquad \ldots(31)$$

Where; y= BOD that has been exerted in time interval t.

K= Reaction rate constant (= K_c).

L= ultimate BOD (the total amount of oxygen consumed when the biochemical reaction is allowed to proceed to completion).

Eq. 32 has a form of straight line equation;

$$Z=a+bt \qquad \ldots(32)$$

where;

$$z = \left(\frac{t}{y}\right)^{\frac{1}{3}} \qquad \ldots(33\text{-a})$$

$$a = (KL)^{-1/3} \qquad \ldots(33\text{-b})$$

$$b= \frac{K^{2/3}}{6L^{1/3}} \qquad \ldots(33\text{-c})$$

and z can be plotted as a function of t. The slope (b) and the intercept (a) of the line of the data best fit can then be used to calculate K and L. To apply this method, a series of BOD measurements verses time are conducted in laboratory, see the results shown in the following table as an example,

Time (day)	0.5	1	2	3	4	5	7	10	15
BOD (mg/l)	5	22	90	160	200	220	260	285	320

Then the following steps are adopted;

1. The BOD values are plotted verses t to determine if the oxygen uptake began immediately or if a lag was evident, see Fig.1 as an example. From Fig.1 it can be shown that the time of beginning which best fits the data is 0.8day. Then, the times of BOD taken are corrected by this amount, as shown in the following table;

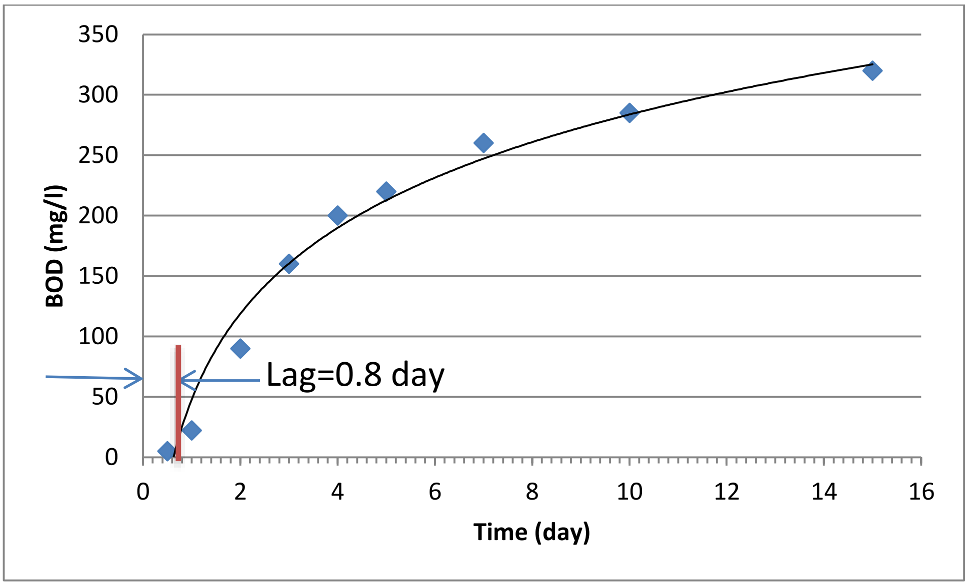


Fig.1 BOD verses t

Time (day)	Corrected time (day)	BOD (mg/l)	$(t/BOD)^{1/3}$
0.5	----	5	----
1	0.2	22	0.21
2	1.2	90	0.24
3	2.2	160	0.24
4	3.2	200	0.25
5	4.2	220	0.27
7	6.2	260	0.29
10	9.2	285	0.32
15	14.2	320	0.35

2. Plot (t/BOD)$^{1/3}$ verses t as shown in Fig.2. From this figure it can be shown that a=0.22 and b=0.0101. then;

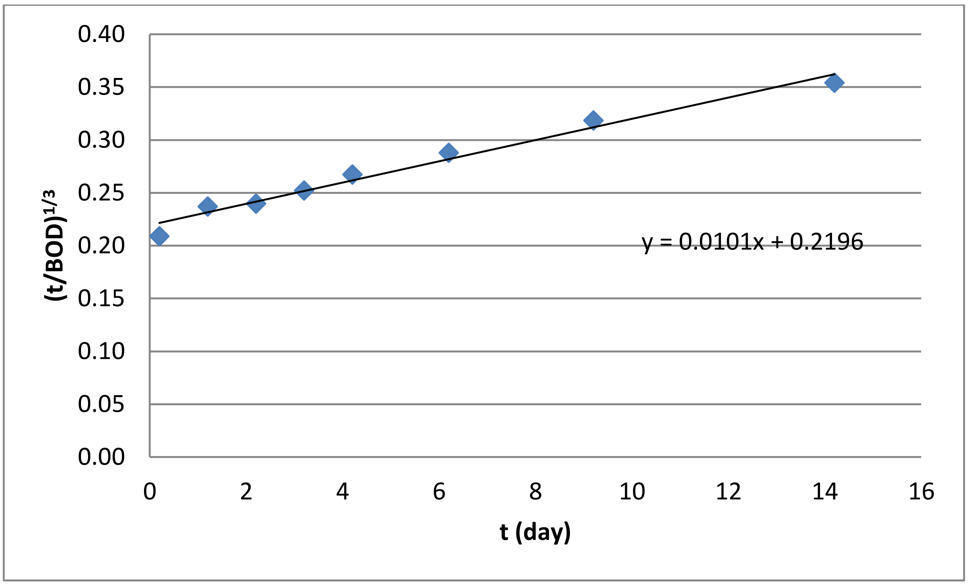


Fig.2 (t/BOD)$^{1/3}$ verses t

$$(KL)^{-1/3} = 0.22 \qquad \ldots(34)$$

$$\frac{K^{2/3}}{6L^{1/3}} = 0.0101 \qquad \ldots(35)$$

Solving Eqs. (34) and (35) give the values of K and L.

Overview on BOD Test

A BOD determination is performed by taking a water sample and incubating it over a 5- or 20-day period while monitoring the dissolved oxygen concentration every 12 hours. In a sample containing high concentrations of BOD, the sample should be diluted to ensure that the original oxygen level present in the water sample is not fully consumed. There are several requirements for the water used in the dilution of the sample. Distilled water should not be used, as microorganisms require certain salts to carry out metabolizes. Thus, potassium, sodium, calcium, magnesium, iron, and ammonium salts are added to the dilution water. Also, the water should be buffered between a pH range of 6.5 to 8.5 with phosphate buffer. In some cases, certain water samples may require a “seed” of viable microorganisms to complete the degradation process. A general rule-of-thumb has been developed to provide sufficient accuracy in determining BOD values. This states that at least 2 mg/L of oxygen must be used over the course of the experiment, but at least 0.5 mg/L must remain in the final sample. The oxygen concentration can be measured by the Winkler Titration Method (for dissolved oxygen concentration), or by utilizing a dissolved oxygen probe. A complete description of the procedure for the handling of samples, making dilution water, incubating samples, and determining oxygen concentration may be found in Standard Methods for the Examination of Water and Wastewater (1998).

7. Volatile Organic Compounds (C_7)

Volatile Organic Compounds (VOCs), such as benzene, methylene chloride, and methyl chloroform are carbon containing compounds that can evaporate into the air at normal temperature. VOCs are commonly found in household and industrial products including gasoline, solvents, cleaners and degreasers, paints, inks and dyes, and pesticides. For example, gasoline is a mixture of VOCs including benzene, toluene, and other hydrocarbons.

The transformation processes that affect the concentration of VOCs in water are; (1) volatilization, (2) hydrolysis, (3) biodegradation, and (4) photolysis. Volatilization is the predominant loss mechanism. Thus, the reaction term of any VOC (R_7) is expressed as;

$$R_7 = -K_V C_7 \qquad \ldots(36)$$

Where; K_V is volatilization rate constant (day^{-1}) which can be calculated as;

$$K_V = COND \times \frac{As}{V} \times f_D \qquad \ldots(37)$$

Where;

COND= conductivity of the compound through the water segment (m/day).

As= surface area of water segment (m^2).

V= volume of the water segment (m^3).

f_D= fraction of compound that is dissolved.

COND value can be obtained as;

$$COND = (R_L + R_G)^{-1} \qquad \ldots(38)$$

Where;

R_L= liquid phase resistance (day/m).

R_G= gas phase resistance (day/m).

The values of R_L and R_G can be obtained as;

$$R_L = \frac{1}{K_a . H \sqrt{\frac{32}{MW}}} \qquad \ldots(39)$$

$$R_G = \frac{1}{\frac{H_C}{R.T} . WAT \sqrt{\frac{18}{MW}}} \qquad \ldots(40)$$

Where;

K_a= reaeration coefficient (day^{-1}).

H= flow depth (m).

MW= molecular weight of compound,

WAT= water vapor exchange constant (m/day).

Hc= Henry's law constant (atm.m^3/mol).

R= ideal gas constant= 8.26×10^{-5} m^3.atm/mol.°K.

T= water temperature (°K).

Hint: Henry's law states that the amount of dissolved gas is proportional to its partial pressure in the gas phase. The proportionality factor is called the Henry's law constant. It was formulated by the English chemist William Henry.

The water vapor exchange constant (WAT) can be estimated as;

$$WAT = 4.46 + 272.7W_{10} \qquad \ldots(41)$$

Where; W10 is the wind speed at 10cm above water surface (m/sec). Wind speed measured above Z, W_Z, can be adjusted to the 10 cm height by the following equation;

$$W_{10} = W_Z \frac{log\frac{0.1}{0.001}}{log\frac{z}{0.001}} \qquad \ldots(42)$$

8. Dissolved Oxygen (C_8)

The primary sources of dissolved oxygen (DO) in a natural water body are; reaeration from the atmosphere and photosynthetic activities of aquatic plants. While, the primary sinks of DO are; respiration requirement of aquatic plants, biochemical oxygen demanding materials and sediment (or benthic) oxygen demand. Fig.1 shows a bock diagram for the sources and sinks of DO in water

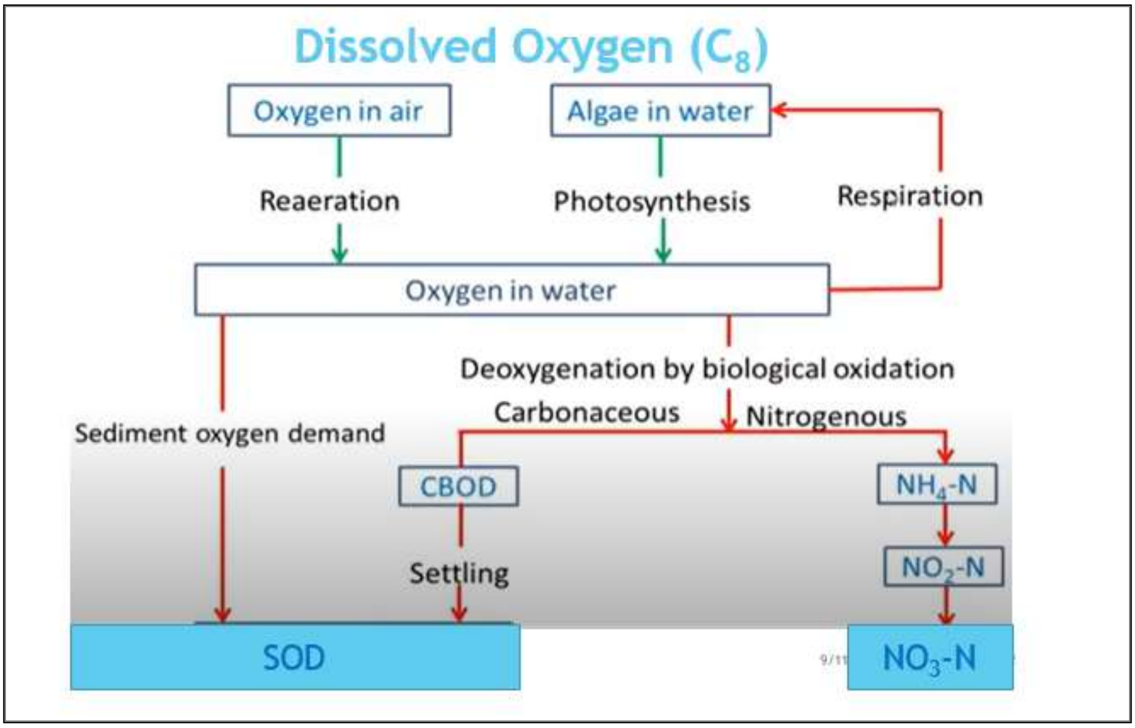


Fig.1 Sources and sinks of DO in surface water

The rate of DO concentration variation due to the combined effects of these processes, R_8, can be expressed as;

$$R_8 = K_a(C_{sat} - C_8) + P - R - B - S_B \qquad \ldots(43)$$

Where;

K_a= reaeration coefficient (day^{-1}).

C_{sat}= saturation value of dissolved oxygen (mg/l).

C_8= DO concentration at specific location and time (mg/l).

P= rate of DO produced by photosynthesis (mg/l/day).

R= rate of DO removed by plant respiration (mg/l/day).

B= rate of DO removed by biological oxidation (mg/l/day).

S_B= rate of DO removed by benthic demand (mg/l/day).

The term $K_a(C_{sat} - C_8)$ on the right hand side of Eq. 43 represents the addition of oxygen by reaeration process which is assumed to be directly proportional to DO deficit, $(C_{sat} - C_8)$. The reaeration coefficient (K_a) can be determined using different equations. In most of these, K_a is related to flow velocity and depth of the stream. For example, if the flow velocity in an estuary varies on the range 0.2-0.58m/sec, K_a is calculated as;

$$K_a = 4.74\left(\frac{U_T}{H}\right)^{0.85} \qquad \ldots(44)$$

Where;

U_T= total flow velocity (m/sec).

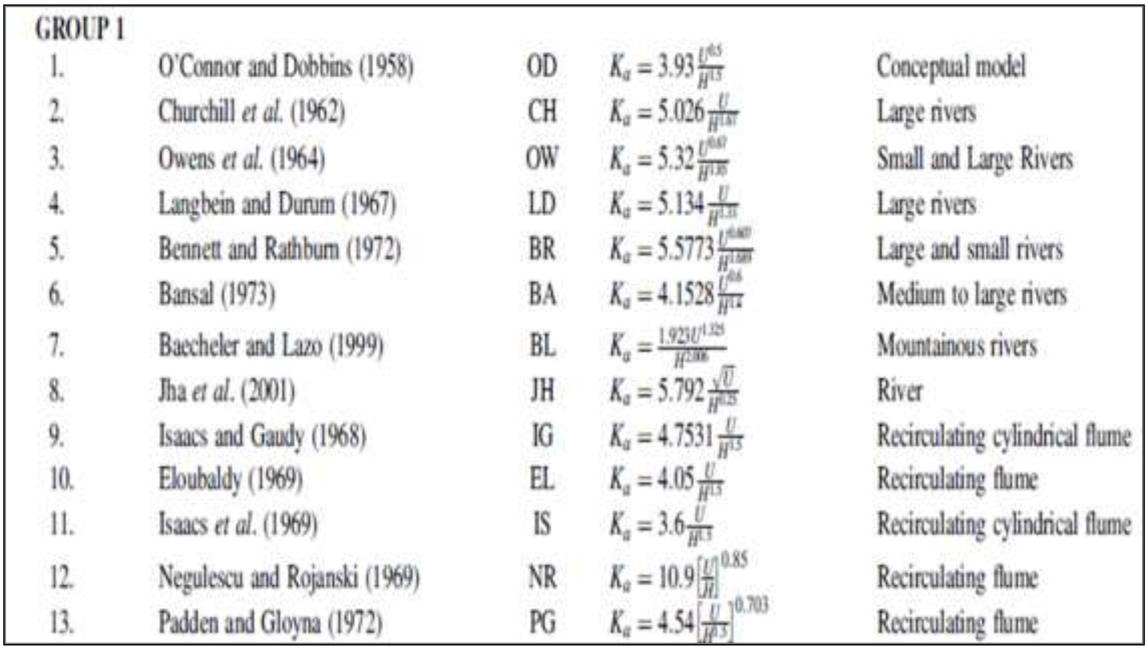
H= flow depth (m).

K_a= reaeration coefficient (day^{-1}) at 20°C.

The value of K_a at any temperature is obtained as;

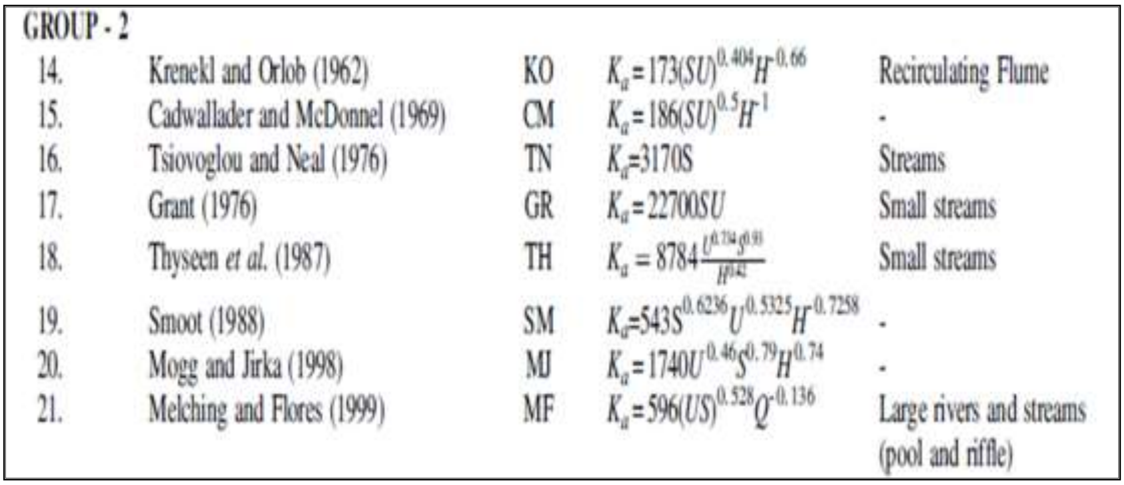
$$K_{a(T^oC)} = K_{a(20^oC)} \times 1.024^{(T-20)} \qquad \ldots(45)$$

In general, the reaeration coefficient equations are classified into three groups. In the first group of equations, K_a depends on flow velocity (U) and flow depth (H). In the second group of equations, K_a depends on U, H, and bottom slope (S). Whereas, in the third group of equations, K_a depends on U, H, S, shear velocity U^* as shown below:



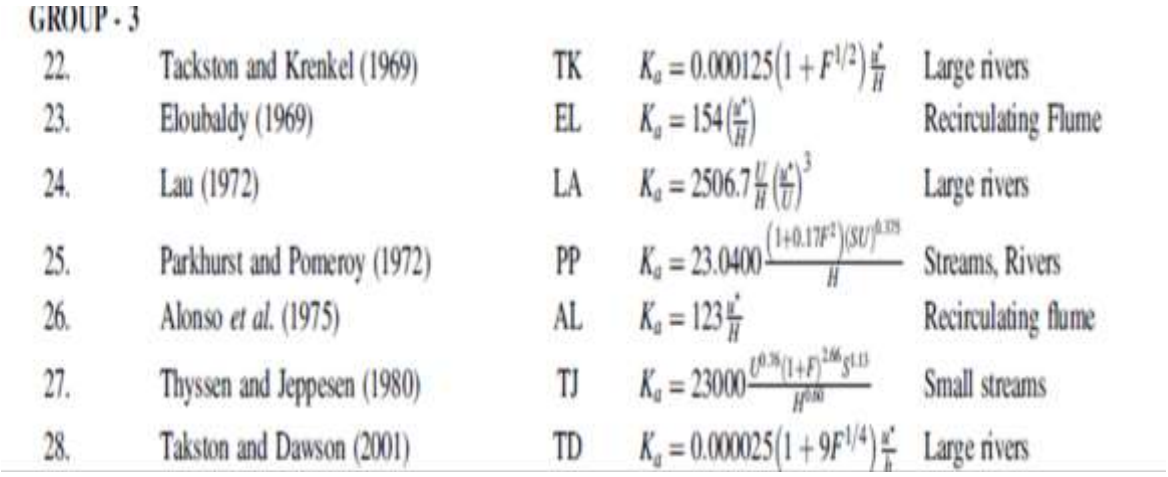
GROUP 1

1.	O'Connor and Dobbins (1958)	OD	$K_a = 3.93\frac{U^{0.5}}{H^{1.5}}$	Conceptual model
2.	Churchill *et al.* (1962)	CH	$K_a = 5.026\frac{U}{H^{1.67}}$	Large rivers
3.	Owens *et al.* (1964)	OW	$K_a = 5.32\frac{U^{0.67}}{H^{1.85}}$	Small and Large Rivers
4.	Langbein and Durum (1967)	LD	$K_a = 5.134\frac{U}{H^{1.33}}$	Large rivers
5.	Bennett and Rathburn (1972)	BR	$K_a = 5.5773\frac{U^{0.607}}{H^{1.689}}$	Large and small rivers
6.	Bansal (1973)	BA	$K_a = 4.1528\frac{U^{0.6}}{H^{1.4}}$	Medium to large rivers
7.	Baecheler and Lazo (1999)	BL	$K_a = \frac{1.923U^{1.325}}{H^{2.006}}$	Mountainous rivers
8.	Jha *et al.* (2001)	JH	$K_a = 5.792\frac{\sqrt{U}}{H^{0.25}}$	River
9.	Isaacs and Gaudy (1968)	IG	$K_a = 4.7531\frac{U}{H^{1.5}}$	Recirculating cylindrical flume
10.	Eloubaldy (1969)	EL	$K_a = 4.05\frac{U}{H^{1.5}}$	Recirculating flume
11.	Isaacs *et al.* (1969)	IS	$K_a = 3.6\frac{U}{H^{1.5}}$	Recirculating cylindrical flume
12.	Negulescu and Rojanski (1969)	NR	$K_a = 10.9\left[\frac{U}{H}\right]^{0.85}$	Recirculating flume
13.	Padden and Gloyna (1972)	PG	$K_a = 4.54\left[\frac{U}{H^{1.5}}\right]^{0.703}$	Recirculating flume



GROUP - 2

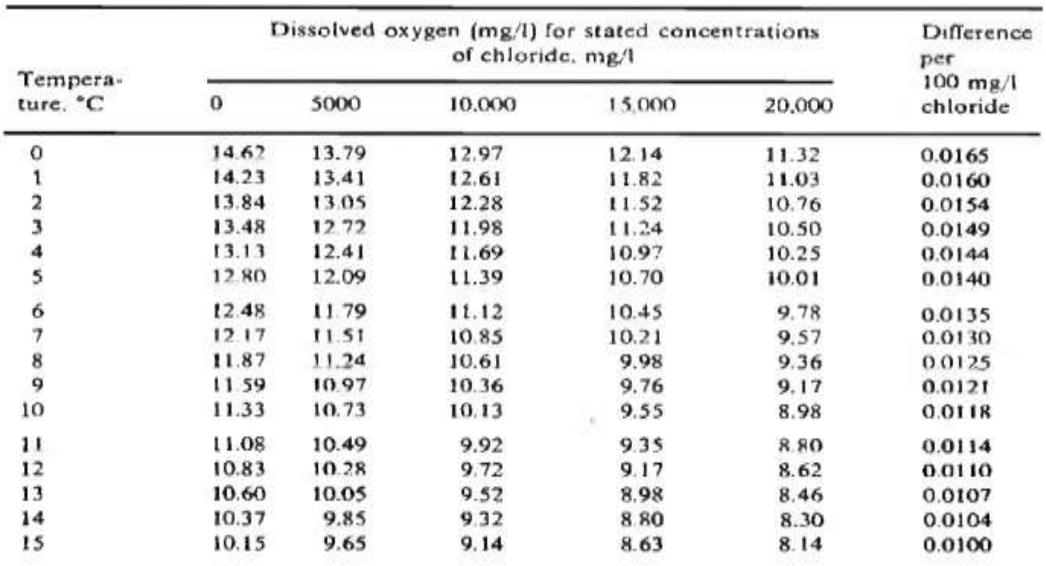
14.	Krenekl and Orlob (1962)	KO	$K_a=173(SU)^{0.404}H^{-0.66}$	Recirculating Flume
15.	Cadwallader and McDonnel (1969)	CM	$K_a=186(SU)^{0.5}H^{-1}$	-
16.	Tsiovoglou and Neal (1976)	TN	$K_a=3170S$	Streams
17.	Grant (1976)	GR	$K_a=22700SU$	Small streams
18.	Thyseen *et al.* (1987)	TH	$K_a = 8784\frac{U^{0.734}S^{0.93}}{H^{0.42}}$	Small streams
19.	Smoot (1988)	SM	$K_a=543S^{0.6236}U^{0.5325}H^{-0.7258}$	-
20.	Mogg and Jirka (1998)	MJ	$K_a=1740U^{0.46}S^{0.79}H^{0.74}$	-
21.	Melching and Flores (1999)	MF	$K_a=596(US)^{0.528}Q^{-0.136}$	Large rivers and streams (pool and riffle)



GROUP - 3

22.	Tackston and Krenkel (1969)	TK	$K_a = 0.000125\left(1+F^{1/2}\right)\frac{u^*}{H}$	Large rivers
23.	Eloubaldy (1969)	EL	$K_a = 154\left(\frac{u^*}{H}\right)$	Recirculating Flume
24.	Lau (1972)	LA	$K_a = 2506.7\frac{U}{H}\left(\frac{u^*}{U}\right)^3$	Large rivers
25.	Parkhurst and Pomeroy (1972)	PP	$K_a = 23.0400\frac{\left(1+0.17F^2\right)(SU)^{0.375}}{H}$	Streams, Rivers
26.	Alonso *et al.* (1975)	AL	$K_a = 123\frac{u^*}{H}$	Recirculating flume
27.	Thyssen and Jeppesen (1980)	TJ	$K_a = 23000\frac{U^{0.76}(1+F)^{2.66}S^{1.13}}{H^{0.80}}$	Small streams
28.	Takston and Dawson (2001)	TD	$K_a = 0.000025\left(1+9F^{1/4}\right)\frac{u^*}{h}$	Large rivers

The saturation value of DO is dependent on water temperature, atmospheric pressure and salinity concentration. For pressure of 101.3 kPa (1 bar), C_{sat} values are presented in the Table below.



Tempera-ture, °C	Dissolved oxygen (mg/l) for stated concentrations of chloride, mg/l					Difference per 100 mg/l chloride
	0	5000	10.000	15.000	20.000	
0	14.62	13.79	12.97	12.14	11.32	0.0165
1	14.23	13.41	12.61	11.82	11.03	0.0160
2	13.84	13.05	12.28	11.52	10.76	0.0154
3	13.48	12.72	11.98	11.24	10.50	0.0149
4	13.13	12.41	11.69	10.97	10.25	0.0144
5	12.80	12.09	11.39	10.70	10.01	0.0140
6	12.48	11.79	11.12	10.45	9.78	0.0135
7	12.17	11.51	10.85	10.21	9.57	0.0130
8	11.87	11.24	10.61	9.98	9.36	0.0125
9	11.59	10.97	10.36	9.76	9.17	0.0121
10	11.33	10.73	10.13	9.55	8.98	0.0118
11	11.08	10.49	9.92	9.35	8.80	0.0114
12	10.83	10.28	9.72	9.17	8.62	0.0110
13	10.60	10.05	9.52	8.98	8.46	0.0107
14	10.37	9.85	9.32	8.80	8.30	0.0104
15	10.15	9.65	9.14	8.63	8.14	0.0100

C_{sat} can be obtained as;

$$C_{sat} = \frac{475-2.65S}{33.5+T} \qquad \ldots(46)$$

where;

T= temperature (°T).
S= salinity (g/kg).
The dependency of C_{sat} on temperature (°C) only is expressed as;

$$C_{sat} = 14.652 - 0.41022T + 0.007991T^2 - 0.000077774T^3 \qquad \ldots(47)$$

Photosynthesis and cellular respiration are two integral processes in the transformation of energy. Aquatic plants use sunlight to convert carbon dioxide (CO_2) and water (H_2O) into glucose ($C_6H_{12}O_6$) for energy. Oxygen (O_2) is produced as a byproduct that is used in aerobic respiration. Aerobic cellular respiration uses O_2 to release energy from glucose molecules and in the process, produces CO_2 as a byproduct. The rate of DO production by photosynthesis, P (mg/l/day), is obtained as;

$$P = 3.16Ch\frac{I^{2/3}}{K_e} + 0.16T - 0.56H \qquad \ldots(48)$$

Where;

Ch= mean chlorophyll concentration (mg/l).

I= mean daily solar intensity (g.cal/cm^2/day).

K_e= light extinction coefficient (1/m).

T= mean temperature (°C).

H= flow depth (m).

The value of P can, also, be obtained using the assimilation number which is defined as the grams of oxygen produced per hour per gram of chlorophyll "a". The values of assimilation number vary over the range (0.7-4.5) g O_2 per hour per g chlorophyll "a".

The rate of DO removed by plants respiration (R) can be obtained as;

$$R = 0.025Ch \qquad \ldots(49)$$

Where R in mg/l/day and Ch in μg/l.

The rate of oxygen removal by biological oxidation (B) is obtained as;

$$B = a_3K_3C_3 + a_4K_4C_4 + K_{c3}C_6 \qquad \ldots(50)$$

where; a_3 and a_4 are stoichiometric constants which specify the number of grams of oxygen consumed in biological oxidation of ammonium-N and nitrite-N, respectively. The values of a_3 and a_4 are;

$$a_3 = 3.43\ g\ O_2\ per\ 1\ g\ NH_4^+ - N$$

$$a_4 = 1.14\ g\ O_2\ per\ 1\ g\ NO_2^- - N$$

Sediment (or benthic) oxygen demand (S_B) is a measure of the DO removed from overlying waters by processes occurring through a unit area of stream bed in unit time. S_B at 20°C (mg/l/day) is determined as;

$$S_B = \frac{1.5\ (g/m^2 per\ day)}{H\ (m)} \qquad \ldots(51)$$

Temperature effect on SB is approximated by;

$$S_{B(T^oC)} = S_{B(20^oC)} \times 1.065^{(T-20)} \qquad \ldots(52)$$

In some of previous studies, it was assumed that algae respiration and photosynthesis production are approximately in balance, and the net effect was assumed to be insignificant by contrast to the other sources and sinks. Other studies represented the net DO production by algae as;

$$P - R = \propto \mu C_{algae} \qquad \ldots(53)$$

where;

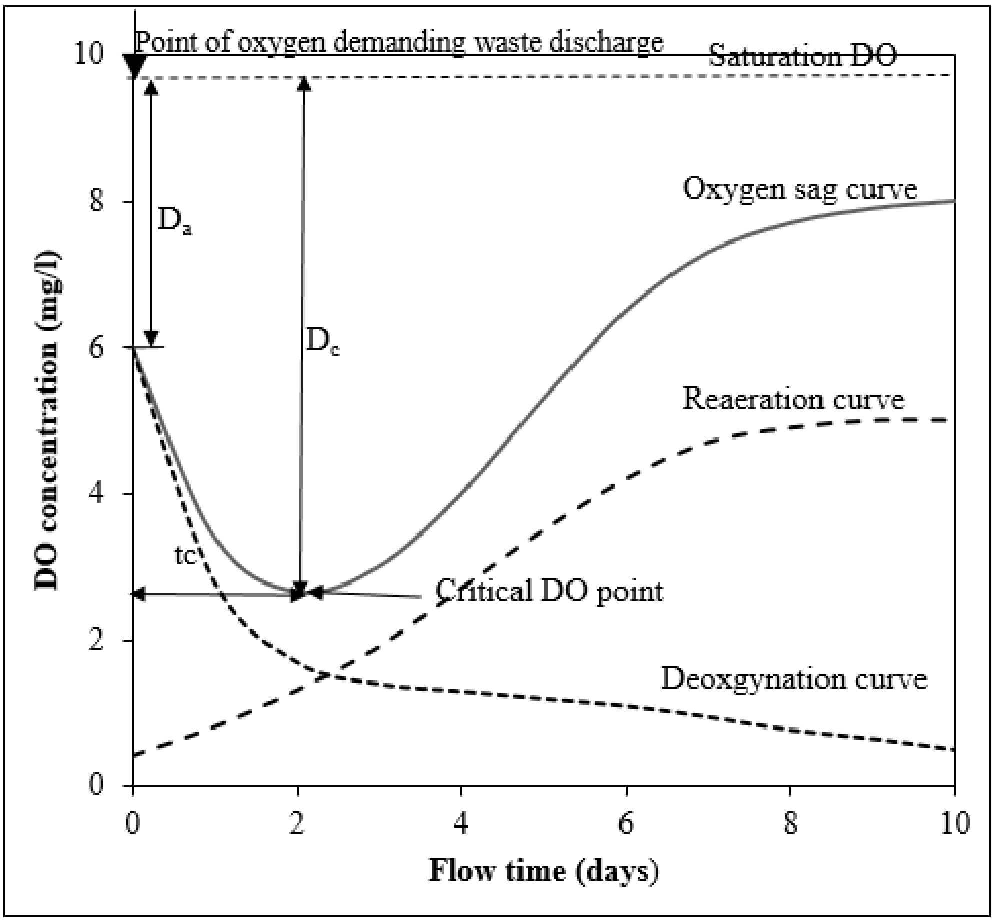
$\propto$ = rate of oxygen mass produced per unit mass of algae growth.

μ= rate of algae growth.

C_{algae}= algae concentration (dry mass/ unit volume of water).

Oxygen Sag Curve

If the stream is originally saturated with DO the BOD uptake curve for the mixture of effluent and stream water gives the cumulative deoxygenation of the stream. As soon as BOD begins to be exerted the DO falls below saturation and reaeration starts. With increasing saturation deficit, the rate of reaeration increases until a critical point is reached where the rates of deoxygenation and reaeration are equal. At the critical point, minimum DO is reached and as further time passes the DO will increase.



Streeter-Phelps equation

Assuming that the only processes involved are BOD removal by biological oxidation and DO replenishment by reaeration from the atmosphere, the Streeter-Phelps equation was derived;

$$\frac{dD}{dt} = K_1L - K_2D$$

Where;

D = DO deficit at time t,

L = ultimate BOD,

K_1 = BOD reaction rate constant

K_2 = reaeration constant.

Oxygen Deficit Equation

Integrating and changing to base 10 (k = 0.4343 K), we get;

$$D_t = \frac{k_1 L_a}{k_2 - k_1}\left(10^{-k_1 t} - 10^{-k_2 t}\right) + D_a 10^{-k_2 t}$$

where Da and La are values at t = 0 and the ultimate BOD remaining at time t is;

$$L_t = L_a 10^{-k_1 t}$$

Maximum Oxygen Deficit

The critical point, i.e. the point of maximum deficit, is given by

$$\frac{dD}{dt} = 0 = K_1L - K_2D$$

Hence

$$D_c = \frac{k_1}{k_2} L_a 10^{-k_1 t_c}$$

$$t_c = \frac{1}{k_2 - k_1} \log \frac{k_2}{k_1}\left[1 - \frac{D_a(k_2 - k_1)}{L_a k_1}\right]$$

where D_c = critical deficit which occurs at time t_c.

9. Chlorophyll "a" (C_9)

In order to consider the effect of aquatic plants activities on DO in surface water, the distribution of chlorophyll concentration in the considered surface water body is needed to be predicted. Chlorophyll is photosynthetic pigment found in plants. Chlorophyll helps in harvesting of solar energy during photosynthesis. There are five types of chlorophyll; a, b, c, d and e. Chlorophyll "a" is found in all types of organisms that use photosynthesis, which includes both land plants and algae. While chlorophyll types b, c, d and e are specific. For examples; Chlorophyll "b" is found in higher plants and green algae, Chlorophyll "c" is found in brown algae and diatoms, Chlorophyll "d" is found in red algae and Chlorophyll "e" is found in golden algae.

Diatoms are a type of unicellular algae. These diatoms range in size from less than 5 μm to more than 100 μm, and have a unique capability of extracting silica from water to produce their skeletal structure. When diatoms die, their skeletons form a diatomite deposit. In its natural state, diatomite is 85% inert silica. The soluble portion of diatomite is extremely low (less than 1%). The odorless, tasteless, and chemically inert characteristics make diatoms safe for filtering water intended for human consumption.

The concentration of chlorophyll a indicates the present of algae and it is progressing proportionally with algae density. Therefore, all the processes that affect algal density will, subsequently, affect chlorophyll a concentration. The reaction term for chlorophyll a is formulated as;

$$R_9 = (G - D - Z)C_9 \qquad \ldots(54)$$

Where;

G= algae growth rate (day^{-1}).

D= endogenous respiration rate (day^{-1}).

Z= grazing rate by zooplankton (day^{-1})

10. Crude Oil (C_{10})

Oil may be released into the marine environment from routine or accidental releases as a result of human activities including drilling, manufacturing, storing, transporting, and waste management. From the time the oil spreads over the water, many physical, chemical, and biological transformation processes occur. These processes include evaporation, dissolution, emulsification, dispersion, biodegradation, oxidation, and sedimentation, Fig.1. these processes are influenced by the following factors:

1- Hydro-meteorological conditions (wave, winds, currents, solar radiation, etc.).
2- Oil properties (density, viscosity, etc.).
3- Oil discharge characteristics (instantaneous, continuous, surface, depth). several processes take place, directly or indirectly related, which disperse the oil and change its properties.

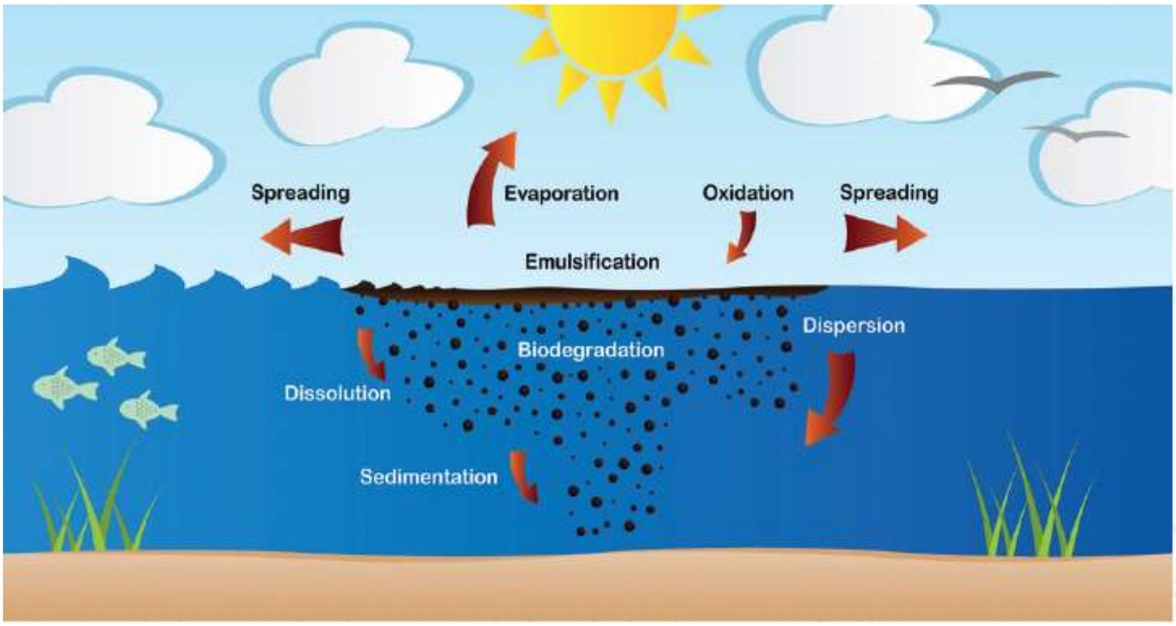


Fig.1 Transformation processes that oil undergoes in the sea

Natural processes can reduce the severity of an oil spill or accelerate the decomposition of spilled oil are described below:

Spreading

The spreading of oil spilled on the sea surface occurs under the influence of gravitation forces. It is controlled by oil viscosity and the surface tension of water. Only ten minutes after a spill of 1 ton of oil, the oil can spread over a radius of 50 m, forming a slick 10-mm thick. The slick gets thinner (less than 1 mm) as oil continues to spread, covering an area of up to 12 km^2.

Drift

Further changes take place under the combined impact of meteorological and hydrological factors and depend mainly on the power and direction of wind, waves, and currents. An oil slick usually drifts in the same direction as the wind.

Dispersion

Winds, waves, and currents may result in natural dispersion, breaking a slick into droplets which are then distributed throughout the water. These droplets may also result in the creation of a secondary slick or thin film on the surface of the water.

Evaporation

Evaporation occurs when the lighter substances within the oil mixture become vapors and leave the surface of the water. This process leaves behind the heavier components of the oil, which may undergo further weathering or may sink to the sea bottom. For example, spills of lighter refined petroleum-based products such as kerosene and gasoline may evaporate completely within a few hours, thereby reducing the toxic effects to the environment. Heavier oils leave a thicker, more viscous residue, which may have serious physical and chemical impacts on the environment.

Emulsification

Emulsification is a process that forms emulsions consisting of a mixture of small droplets of oil and water. Emulsions are formed by wave action, and greatly hamper weathering and cleanup processes. Two types of emulsions exist: water-in-oil and oil-in-water. Water-in-oil emulsions are frequently called “chocolate mousse,” and they are formed when strong currents or wave action causes water to become trapped inside viscous oil. Chocolate mousse emulsions may remain in the environment for months or even years. Oil and water emulsions cause oil to sink and disappear from the surface, which give the false impression that it is gone and the threat to the environment has ended.

Biodegradation

Biodegradation occurs when microorganisms such as bacteria feed on oil. A wide range of microorganisms is required for a significant reduction of the oil.

To sustain biodegradation, nutrients such as nitrogen and phosphorus are sometimes added to the water to encourage the microorganisms to grow and reproduce. Biodegradation tends to work best in warm water environments.

Photo-Oxidation

Chemical transformations of oil on the water surface and in the water column mainly have an oxidative nature and often involve photochemical reactions under the influence of ultraviolet waves of the solar spectrum. The final products of oxidation usually have increased water solubility. An experimental research showed that they have increased toxicity as well.

Sedimentation

Some of the oil (up to 10-30%) is adsorbed on the suspended material and deposited to the bottom. This mainly happens in the narrow coastal zone and shallow waters where suspended solids concentration is high and water is subjected to intense mixing. In deeper areas remote from the shore, sedimentation of oil (except for the heavy fractions) is an extremely slow process.

Dissolution

Most oil components are water-soluble to a certain degree, especially low-molecular-weight hydrocarbons. Hydrodynamic and physicochemical conditions in the surface waters strongly affect the rate of the process.

Duration of oil transformation processes

All of oil slick transformation processes are time dependent. However their durations of occurrence differ as shown in Fig.2. The chart in Fig.2 shows duration of oil slick processes in the sea. In this chart, the vertical axis represents the physicochemical processes that oil is going through, and the time each one of them requires is depicted in the horizontal axis, whereas the line thickness denotes the most critical phase of each stage.

In general, transformation processes such as spreading, evaporation, dissolution, dispersion, and emulsification are rapidly occurring (within hours) and have immediate effects on the oil slick. Sedimentation, biodegradation and photo-oxidation operate more slowly (within months) and comprise the long-term mechanisms for the breakdown of hydrocarbons in the environment.

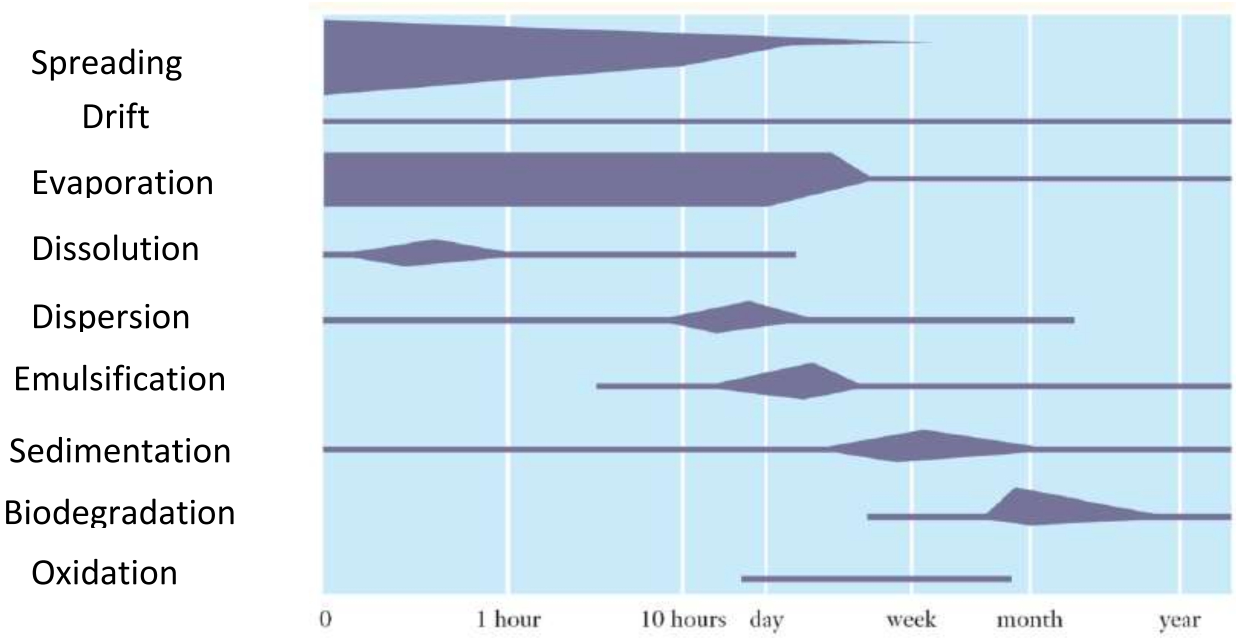


Fig.2 Duration of oil slick processes in the sea

11. Heavy metals (C_{11})

Heavy metal (such as zinc, iron, lead, cadmium and nickel) inputs to surface waters include those from commercial fertilizers, liming materials and agrochemicals, sewage sludge and other wastes used as soil amendments, irrigation waters, and atmospheric deposition. Upon entry into surface waters, heavy metals deposition occurs on the bottom of aquatic areas
(streams, lakes, estuaries).

Rivers passing through industrial and mining areas transport metals, partly as metal in solution and partly as metal adsorbed to suspended material. This suspended material settles to the bottom of lakes and estuaries and accumulates in the sediment. Aquatic organisms may be adversely affected by heavy metals in the environment. The toxicity is largely a function of the water chemistry and sediment composition in the surface water system. Metals may enter the aquatic organisms via three main pathways:

1. Free metal ions that are absorbed through respiratory surface (e.g., gills) are readily diffused into the blood stream.
2. Free metal ions that are adsorbed onto body surfaces are passively diffused into the blood stream.
3. Metals that are sorbed onto food and particulates may be ingested, as well as free ions ingested with water.

It is assumed that the metals are distributed homogeneously in the water column as well as in the upper sediment layer. In both compartments, the metals with total concentration of C_T can exist in either a dissolved form (with concentration C_D) or adsorbed to solid particles (with concentration C_A), both in the water column or in the top layer of sediment (Eqs. 55-60).

$$C_T = C_D + C_A \qquad (1)$$

$$C_D = f_D\, C_T \qquad (2)$$

$$C_{D1} = f_{D1}\, C_{T1} \qquad (3)$$

$$C_{D2} = f_{D2}\, C_{T2} \qquad (4)$$

$$C_{A1} = (1\text{-}f_{D1})\, C_{T1} \qquad (5)$$

$$C_{A2} = (1\text{-}f_{D2})\, C_{T2} \qquad (6)$$

The dissolved fraction, f_D, is given by the distribution coefficient, K_D (Eqs. 7-9):

$$f_D = \frac{1}{1 + mK_D} \qquad (7)$$

$$f_{D1} = \frac{1}{1 + mK_{D1}} \qquad (8)$$

$$f_{D2} = \frac{1}{1 + mK_{D2}} \qquad (9)$$

where m is the total concentration of the suspended particles.

The rate of sedimentation of suspended particles settling with velocity vs is given by Eq (10).

$$J_s = v_s\, A\, C_A = v_s\, A\, (1 - f_D)\, C_T \qquad (10)$$

The particles in the top layer of sediment also settle until they reach a certain depth at which they are no longer influenced by the water column. Due to differences in the dissolved metal concentration in the water column and in the top layer of the sediment, a diffusion exchange between the two compartments will occur, proportional to the difference in concentration and the area of the sediment-water interface. This exchange is defined by the proportionality constant K_L (Eq. 11).

$$J_d = K_L\, A\, (C_{D1} - C_{D2}) \qquad (11)$$

12. Phosphate-P (C_{12})

The concentration of phosphate-P in natural streams decreases due to settling process to bottom sediments and increases due to decomposition of algae. Thus, the reaction term (R_{12}) can be formulated as;

$$R_{12} = -K_S C_{12} + r_p (D + 0.4Z) C_9 \qquad \ldots(55)$$

Where;

K_s= rate coefficient of settling= 0.01/day.

r_p= phosphate- chlorophyll "a" ratio.

D= endogenous respiration rate (day^{-1}).

Z= grazing rate by zooplankton (day^{-1}).

The highest values of r_p can be 0.02 mg of phosphorus per mg of algae, as observed when a poor sunlight and a low water temperature limit the growth of algae cells.

3D Flow Model

Navier-Stokes Equations

It is well known that the most general equations for a viscous incompressible fluid are momentum equations in x-, y- and z- directions which are known as Navier- Stokes equations;

Momentum equation in x-direction;

(A) (B) (C) (D) (E) (F) (G)

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+\mathrm{v}\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}-f\,\mathrm{v}+\frac{1}{\rho}\frac{\partial P}{\partial x}-\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)=0 \quad \ldots(1)$$

Momentum equation in y-direction;

$$\frac{\partial \mathrm{v}}{\partial t}+u\frac{\partial \mathrm{v}}{\partial x}+\mathrm{v}\frac{\partial \mathrm{v}}{\partial y}+w\frac{\partial \mathrm{v}}{\partial z}+f\,u+\frac{1}{\rho}\frac{\partial P}{\partial y}-\nu\left(\frac{\partial^2 \mathrm{v}}{\partial x^2}+\frac{\partial^2 \mathrm{v}}{\partial y^2}+\frac{\partial^2 \mathrm{v}}{\partial z^2}\right)=0 \quad \ldots(2)$$

Momentum equation in z-direction;

$$\frac{\partial \mathrm{w}}{\partial t}+u\frac{\partial \mathrm{w}}{\partial x}+\mathrm{v}\frac{\partial \mathrm{w}}{\partial y}+w\frac{\partial \mathrm{w}}{\partial z}+g+\frac{1}{\rho}\frac{\partial P}{\partial z}-\nu\left(\frac{\partial^2 \mathrm{w}}{\partial x^2}+\frac{\partial^2 \mathrm{w}}{\partial y^2}+\frac{\partial^2 \mathrm{w}}{\partial z^2}\right)=0 \quad \ldots(3)$$

To above equations, a continuity equation is added to introduce the mass conservation principle that when a fluid has a constant density;

$$\frac{\partial \mathrm{u}}{\partial x}+\frac{\partial \mathrm{v}}{\partial y}+\frac{\partial \mathrm{w}}{\partial z}=0 \qquad \ldots(4)$$

Where;

u, v and w= velocity components in x-, y- and z- directions, respectively.

p= pressure.

f= Coriolis parameter which is defined as;

$$f = 2\Omega sin\emptyset$$

Where;

Ω= angular velocity of the earth = $7.3 \times 10^{-5}\ s^{-1}$.

Φ= latitude of the stream.

v= kinematic viscosity of water.

The terms (A), (B), (C) and (D) give the creeping flow, the term (E) gives the mass forces due to gravity and Coriolis accelerations. The terms (F) and (G) are the surface forces due to pressure and viscosity of water. Coriolis acceleration results from earth rotation, by which all horizontally moving objects not subject to any force will accelerate to the right (lift) of their direction of motion in Northern (Southern) hemisphere, see Fig.1.

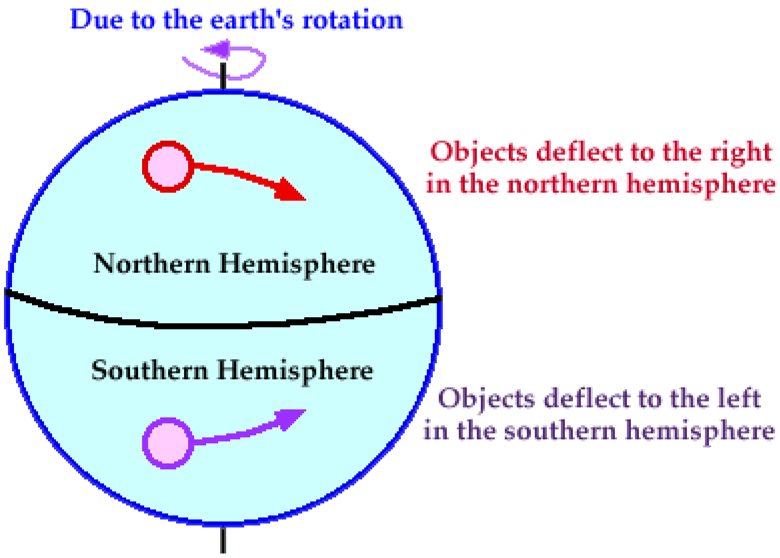


Fig.1 Coriolis acceleration

Reynolds-averaged Navier–Stokes Equations

Reynolds-averaged Navier–Stokes equations (or RANS equations) are time-averaged equations of motion for turbulent fluid flow. The idea behind the equations is Reynolds decomposition, whereby any instantaneous quantity in Navier- Stokes equations, such as u, is decomposed into its time-averaged and fluctuating (due to turbulence) quantities;

$$u = \bar{u} + \grave{u}$$

Where $\bar{u}$ and $\grave{u}$ are the mean and fluctuating values of u, respectively. If a period T is long enough with respect to the fluctuating;

$$\int_T \grave{u} dt = 0$$

and by considering $\frac{\overline{\partial u}}{\partial t} = \frac{\partial \bar{u}}{\partial t}$, RANS equations are obtained;

$$\frac{\partial \bar{u}}{\partial t} + \bar{u}\frac{\partial \bar{u}}{\partial x} + \bar{\mathrm{v}}\frac{\partial \bar{u}}{\partial y} + \bar{w}\frac{\partial \bar{u}}{\partial z} - f\bar{\mathrm{v}} + \frac{1}{\rho}\frac{\partial \bar{P}}{\partial x} - \nu\nabla^2\bar{u} + \left(\frac{\partial}{\partial x}\overline{\grave{u}\grave{u}} + \frac{\partial}{\partial y}\overline{\grave{u}\grave{\mathrm{v}}} + \frac{\partial}{\partial z}\overline{\grave{u}\grave{w}}\right) = 0 \qquad \ldots(5)$$

$$\frac{\partial \bar{\mathrm{v}}}{\partial t} + \bar{u}\frac{\partial \bar{\mathrm{v}}}{\partial x} + \bar{\mathrm{v}}\frac{\partial \bar{\mathrm{v}}}{\partial y} + \bar{w}\frac{\partial \bar{\mathrm{v}}}{\partial z} + f\bar{u} + \frac{1}{\rho}\frac{\partial \bar{P}}{\partial y} - \nu\nabla^2\bar{\mathrm{v}} + \left(\frac{\partial}{\partial x}\overline{\grave{\mathrm{v}}\grave{u}} + \frac{\partial}{\partial y}\overline{\grave{\mathrm{v}}\grave{\mathrm{v}}} + \frac{\partial}{\partial z}\overline{\grave{\mathrm{v}}\grave{w}}\right) = 0 \qquad \ldots(6)$$

$$\frac{\partial \bar{w}}{\partial t} + \bar{u}\frac{\partial \bar{w}}{\partial x} + \bar{\mathrm{v}}\frac{\partial \bar{w}}{\partial y} + \bar{w}\frac{\partial \bar{w}}{\partial z} + g + \frac{1}{\rho}\frac{\partial \bar{P}}{\partial z} - \nu\nabla^2\bar{w} + \left(\frac{\partial}{\partial x}\overline{\grave{w}\grave{w}} + \frac{\partial}{\partial y}\overline{\grave{w}\grave{\mathrm{v}}} + \frac{\partial}{\partial z}\overline{\grave{w}\grave{w}}\right) = 0 \qquad \ldots(7)$$

The RANS equations coincide with the original Navier-Stokes equations having substituted instance value f with mean value $\bar{f}$ and adding a group of terms containing the temporal average of products of rate's fluctuations. These terms have the same structure of viscosity stress terms. Thus they are considered as stresses due to turbulence (turbulence shear stresses) defined as;

$$\frac{\overline{\tau_{ij}}}{\rho} = -\overline{\grave{u}_i\grave{u}_j} \qquad \ldots(8)$$

Eqs. 5, 6 and 7 can be written in terms of turbulent shear stresses as;

$$\frac{\partial \bar{u}}{\partial t}+\bar{u}\frac{\partial \bar{u}}{\partial x}+\bar{\mathrm{v}}\frac{\partial \bar{u}}{\partial y}+\bar{w}\frac{\partial \bar{u}}{\partial z}-f\bar{\mathrm{v}}+\frac{1}{\rho}\frac{\partial \bar{P}}{\partial x}-v\nabla^2\bar{u}-\frac{1}{\rho}\left(\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{xy}}{\partial y}+\frac{\partial \tau_{xz}}{\partial z}\right)=0 \quad \ldots(9)$$

$$\frac{\partial \bar{v}}{\partial t}+\bar{u}\frac{\partial \bar{v}}{\partial x}+\bar{v}\frac{\partial \bar{v}}{\partial y}+\bar{w}\frac{\partial \bar{v}}{\partial z}+f\bar{u}+\frac{1}{\rho}\frac{\partial \bar{P}}{\partial y}-v\nabla^2\bar{v}+-\frac{1}{\rho}\left(\frac{\partial \tau_{yx}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{yz}}{\partial z}\right)=0 \quad \ldots(10)$$

$$\frac{\partial \bar{w}}{\partial t}+\bar{u}\frac{\partial \bar{w}}{\partial x}+\bar{\mathrm{v}}\frac{\partial \bar{w}}{\partial y}+\bar{w}\frac{\partial \bar{w}}{\partial z}+g+\frac{1}{\rho}\frac{\partial \bar{P}}{\partial z}-v\nabla^2\bar{w}+-\frac{1}{\rho}\left(\frac{\partial \tau_{zx}}{\partial x}+\frac{\partial \tau_{zy}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}\right)=0 \quad \ldots(11)$$

Turbulent shear stresses are defined as;

$$\frac{\overline{\tau_{ij}}}{\rho}=\varepsilon_{ij}\left(\frac{\partial \overline{u_i}}{\partial x_j}+\frac{\partial \overline{u_j}}{\partial x_i}\right) \quad \ldots(12)$$

The coefficient ε_{ij} by analogy is called turbulent viscosity but it is not a constant characteristic of a fluid but it is a tensor on account of the characteristic of motion. *Hint: the value of* ε_{ij} *is obtained using suitable turbulence model.*

Equations 9, 10 and 11 with applying a suitable turbulence model are used to compute u, v and w values necessary to solve the 3D transport equation and obtain the 3D distribution of different constituent's concentrations in surface water bodies.

2D Plan View Flow Model

For mainly horizontal motions, vertical acceleration can be neglected. So, Eq.11 is transformed into hydrostatic equation;

$$g+\frac{1}{\rho}\frac{\partial \bar{P}}{\partial z}=0 \quad \ldots(13)$$

Eq.13 expresses a linear variation of the pressure with elevation as in stationary fluids. By neglecting the viscous stresses (their magnitudes are insignificant as compared with turbulent stresses), Eqs. 9 and 10 will become;

$$\frac{\partial \bar{u}}{\partial t}+\bar{u}\frac{\partial \bar{u}}{\partial x}+\bar{\mathrm{v}}\frac{\partial \bar{u}}{\partial y}+\bar{w}\frac{\partial \bar{u}}{\partial z}-f\bar{\mathrm{v}}+\frac{1}{\rho}\frac{\partial \bar{P}}{\partial x}-\frac{1}{\rho}\left(\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{xy}}{\partial y}+\frac{\partial \tau_{xz}}{\partial z}\right)=0\,..(14)$$

$$\frac{\partial \bar{v}}{\partial t}+\bar{u}\frac{\partial \bar{v}}{\partial x}+\bar{v}\frac{\partial \bar{v}}{\partial y}+\bar{w}\frac{\partial \bar{v}}{\partial z}+f\bar{u}+\frac{1}{\rho}\frac{\partial \bar{P}}{\partial y}-\frac{1}{\rho}\left(\frac{\partial \tau_{yx}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{yz}}{\partial z}\right)$$
$$=0\,..(15)$$

The time averaged form of continuity equation is;

$$\frac{\partial \bar{\mathrm{u}}}{\partial x}+\frac{\partial \bar{\mathrm{v}}}{\partial y}+\frac{\partial \bar{\mathrm{w}}}{\partial z}=0 \qquad \ldots(16)$$

It is possible to reduce the three spatial variables (x, y and z) to two variables (x and y) by the method of vertical integration. By vertical integration of Eqs. 14 and 15 and applying boundary conditions on stream bottom and water surface, these equations are written as;

$$\frac{\partial U}{\partial t}+U\frac{\partial U}{\partial x}+V\frac{\partial U}{\partial y}-fV+g\frac{\partial h}{\partial x}-\frac{KW^2}{H}\cos\Psi+\frac{gU(U^2+V^2)^{0.5}}{HC^2}=0$$

…(16)

$$\frac{\partial V}{\partial t}+U\frac{\partial V}{\partial x}+V\frac{\partial V}{\partial y}+fV+g\frac{\partial h}{\partial y}-\frac{KW^2}{H}\sin\Psi+\frac{gV(U^2+V^2)^{0.5}}{HC^2}=0$$

…(17)

Where;

U and V= depth averaged velocity components in x and y directions, respectively, (m/sec)

g= gravity acceleration (m/sec^2).

h= water surface elevation measured from mean sea level (m).

K = dimensionless coefficient that is a function of wind speed.

W= wind velocity (m/sec).

Ψ = the angle between the wind velocity vector and the x axis.

H= total flow depth (m) which is equal to h+b and it is a function of x, y and t.

b= bottom elevation measured from mean sea level and it a function of x and y.

C= Chezy coefficient ($m^{0.5}$/sec)

The depth averaged form of continuity equation is;

$$\frac{\partial h}{\partial t}+\frac{\partial (HU)}{\partial x}+\frac{\partial (HV)}{\partial y}=0 \qquad \ldots(18)$$

The sixth term in each of Eqs. 16 and 17 represents the wind stress. This term is significant in open seas and oceans. In other surface water bodies, the wind stress is insignificant as compared with shear stress at the bottom. Thus, the wind stress term is usually neglected.

Boundary conditions

Equations 16, 17 and 18 are solved simultaneously to get the values of U (x, y, t), V (x, y, t) and h (x, y, t) which are required to simulate constituents distribution using plan view model. The boundary conditions required to solve these equations are;

At solid boundaries;

At solid boundaries, either no-slip or slip boundary conditions are applied.

a. No-slip Boundary condition;

In this case all velocity components are set to be zero;

U=V=0

b. Slip boundary condition;

The velocity component normal to the solid boundary is set to be zero;

$$V_n = U\cos\theta + V\sin\theta$$

Where; V_n is the velocity component normal to the solid boundary and θ is the angle between the x-axis and the outward normal to the boundary.

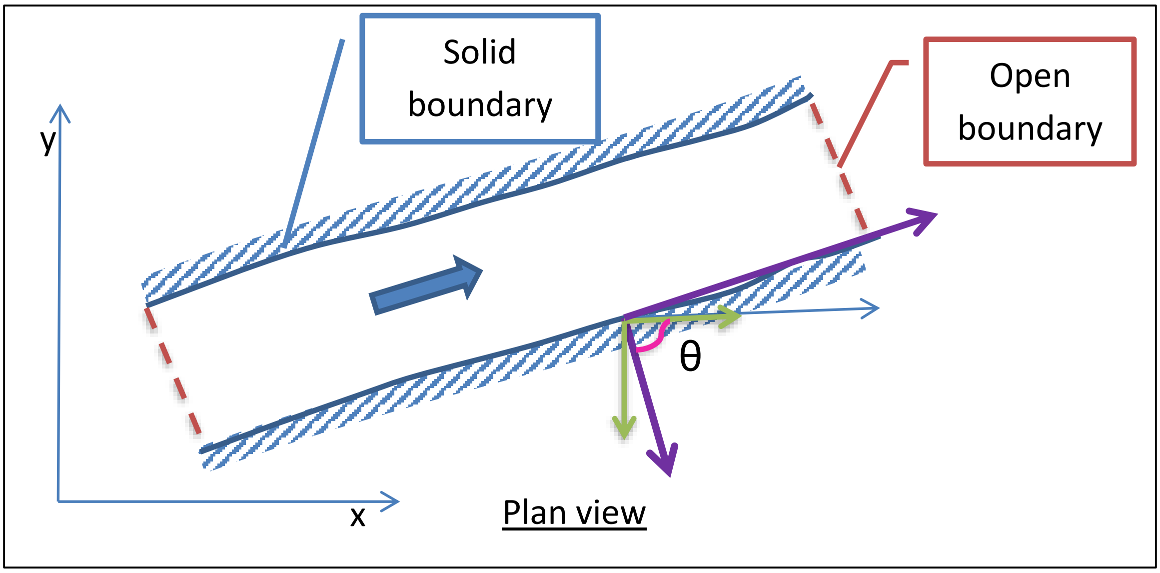


Fig.2 Plan view of stream

At open boundaries;

At open boundaries, either the water level or normal velocity component is specified as a function of time.

2D Side Elevation Flow Model

To develop a 2D side elevation (laterally averaged) flow model, the following assumptions are made:

1. The x-axis is taken along the central stream–line of the estuary at mean sea level (MSL), and the z-axis vertical (positive up ward), Fig.1.

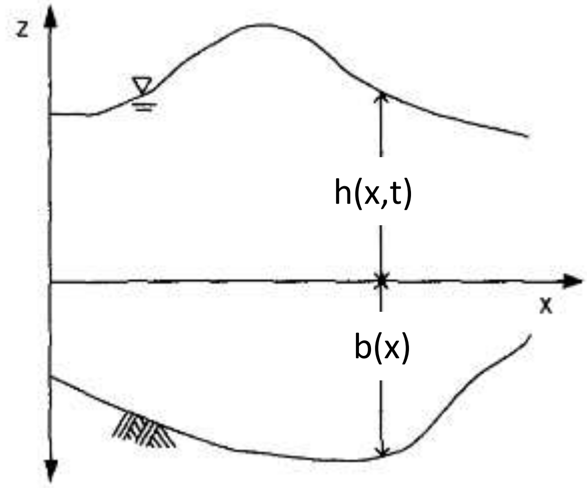


Fig.1 Longitudinal cross section in an estuary

2. The pressure is hydrostatic, because the longitudinal velocity component is several orders of magnitude larger than the vertical component.
3. The total water depth (H) can be represented as;

$$H = h + b$$

where;

h = water surface elevation above MSL

b = bottom depth measured from MSL

4. Neglecting the effect of wind.

The Basic Equations

The basic equations of the model are provided by laterally integrating conservation laws for mass (water), momentum, and salinity concentration.

After integration over the width and if the shallow water approximation is made, the equations for vertical 2D model are:

Momentum equation in x- direction:

$$\frac{\partial}{\partial t}\left(BU\right)+\frac{\partial}{\partial x}(BUU)+\frac{\partial}{\partial z}(BUW)+\frac{\partial}{\partial x}\left(B\tau_{xx}\right)+\frac{\partial}{\partial z}\left(B\tau_{xz}\right)+\tau_{bx}+\frac{B}{\rho_o}\frac{\partial P}{\partial x}=0 \quad ...(1)$$

Momentum equation in z- direction:

With the hydrostatic pressure assumption, the only significant contribution from the vertical momentum equation comes from the gravity acceleration term and is reduction to a hydrostatic pressure distribution.

$$\frac{\partial P}{\partial z}=-\rho g \quad ...(2)$$

In some references, Eq. 2 is defined as;

$$\frac{\partial P}{\partial z}=-\rho g \cos \alpha$$

Define α and why cos α is included in Eq.2?

Continuity equation:

$$\frac{\partial}{\partial x}(BU)+\frac{\partial}{\partial z}(BW)=0 \quad ...(3)$$

Salinity transport equation:

$$\frac{\partial(BS)}{\partial t}+\frac{\partial(BUS)}{\partial x}+\frac{\partial(BWS)}{\partial z}-\frac{\partial}{\partial x}\left(BK_X\frac{\partial S}{\partial x}\right)-\frac{\partial}{\partial y}\left(BK_Z\frac{\partial C}{\partial z}\right)=0 \quad \ldots(4)$$

State equation:

$$\rho=\rho_o(1+\alpha S) \quad \ldots(5)$$

Where;

S= width averaged salinity concentration, mg/l.

U and W= width averaged flow velocity components in x- and z- directions, respectively, m/sec.

K_x and K_z= dispersion coefficients in x- and z- directions, respectively, m^2/sec.

B= stream width witch is a function of x and z.

$\tau_{bx} =$ bottom shear stress.

τ_{xx} *and* τ_{xz} = width averaged turbulent shear stresses

ρ and ρ_o=salted and fresh water densities, respectively.

g= gravity acceleration.

α= constant relating salinity concentration and density. It equals to 0.00075.

The bottom shear stress can be specified follows the well- known quadratic friction law:

$$\tau_{bx} = \frac{g}{C^2} \rho U \left| U \right| \qquad ...(6)$$

in which C is the friction coefficient (Chezy coefficient). Integrating Eq.2 and using Eq.5 results in:

$$P = \rho_0 g(h - z) + \rho_0 g\alpha \int_Z^h S \ dz \qquad ...(7)$$

where h is water surface elevation above the MSL. Differentiating Eq.7 with respect to x gives the pressure gradient in x direction as:

$$\frac{1}{\rho_0} \frac{\partial P}{\partial x} = g \frac{\partial h}{\partial x} + g\alpha \frac{\partial}{\partial x} \int_b^h S dz \qquad ...(8)$$

To calculate the water surface elevation, Eq.3 is integrated vertically (over the depth). After using the Kinematic condition:

$$U \frac{\partial b}{\partial x} \text{-} W = o \qquad (z = b) \qquad ...(9a)$$

and

$$\frac{\partial h}{\partial t} + U \frac{\partial h}{\partial x} \text{-} W = o \qquad (z = h) \qquad ...(9b)$$

Eq.3 becomes:

$$B_h \frac{\partial h}{\partial t} + \int_b^h B \frac{\partial U}{\partial x} dz = 0 \quad ...(10)$$

Where Bh is stream width at the free surface (z=h)

The Turbulence Model

To close the system of equations given above, a turbulence model is necessary. The simplest approach is the eddy viscosity/ diffusivity concept which is a zero- equation method. This approach yields the horizontal and vertical turbulent exchange of momentum and mass respectively:

$$\tau_{xz} = -\varepsilon_z \frac{\partial U}{\partial z} \quad ...(11a)$$

$$\tau_{xx} = -\varepsilon_x \frac{\partial U}{\partial x} \quad ...(11b)$$

where;

ε_x and ε_z = turbulent exchange coefficient for momentum in the x- and z-direction, respectively.

The vertical turbulent exchange coefficient of momentum (ε_z) is determined by using the concept of eddy viscosity with the mixing length model. If mixing length approach is used:

$$\varepsilon_z = l_m^2 \left| \frac{\partial U}{\partial z} \right| \quad ...(12)$$

The mixing length (l_m) is defined as:

$$l_m = k(z + z_0) \quad for.....0 \le z \le 0.25H \quad ...(13a)$$

$$l_m = k(0.25H + z_0) \quad for \quad 0.25H \le z \le H \quad ...(13b)$$

Where; z_0 is a measure for the roughness length and H denotes the water depth.

Boundary Conditions

In developing a two dimensional laterally averaged model, boundary conditions are specified at; (1) free water surface, (2) bottom of estuary (solid boundary),

(3) upstream border and (4) seaward boundary of the simulated estuary. At each boundary, the applied boundary conditions are;

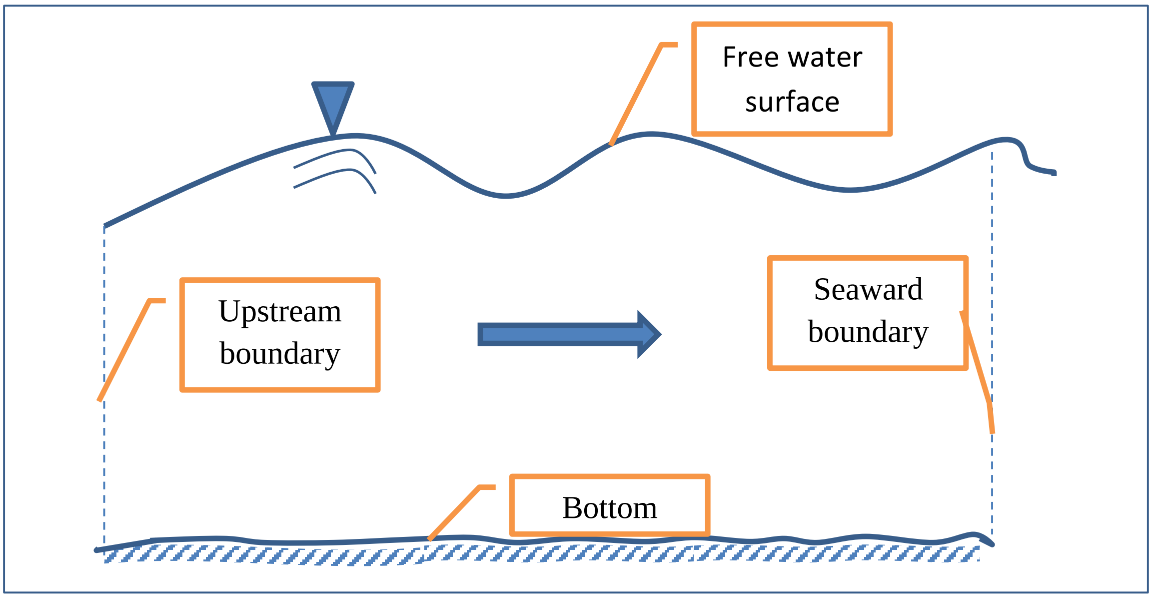


Fig.2 Vertical profile in an estuary

Free surface condition

At the free surface the Kinematic condition holds Eq.9b which was used for the derivation of Eq.10. For the momentum equation, the boundary condition is:

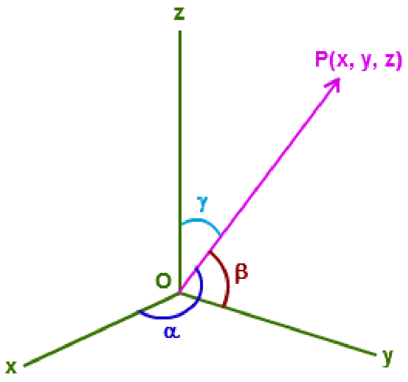
$$\frac{\partial U}{\partial n} = \varepsilon_x \frac{\partial U}{\partial x} l_x + \varepsilon_z \frac{\partial U}{\partial z} l_z = 0 \qquad (no\ wind) \qquad ...(14)$$

where l_x and l_z are the directional cosines

For the transport equation of salinity, the following condition is specified;

$$\frac{\partial s}{\partial n} = K_x \frac{\partial s}{\partial x} l_x + K_z \frac{\partial s}{\partial z} l_z = 0 \qquad ..(15)$$

Direction Cosines: the cosines of the angles made by a directed line segment with the coordinate axes are called as the direction cosines of that line. If α, β, and γ are the angles made by the line segment with the coordinate axis then these angles are termed to be the direction angles and the cosines of these angles are the direction cosines of the line. Hence, cos α, cos β and cos γ .



Bottom condition

The bottom is treated as an impermeable (No- slip boundary) at which (U=W=0). For the transport equation, a condition is specified similar to the one at the surface Eq.15, which means no transport of salinity through the bottom.

Seaward boundary

At the seaward boundary, the surface elevation must be specified;

$$h(z,t) = f(t) \qquad \text{at } x=L \qquad \ldots(16)$$

A condition for the conservation of salt content must be given. During flood tide the increase of the concentration is specified as a function of t and z. During ebb tide a weak condition can be imposed. However, for salinity;

$$S(z,t) = g(z,t) \qquad \text{at } x = L \qquad \ldots(17)$$

Upstream boundary

At the upstream boundary of the estuary, the following conditions are valid;

For the velocities;

$$U(z,t)= U_0(t,z) \quad \text{at } x = o \qquad \ldots(18)$$

For the water level;

$$h(z,t)=h_o \quad \text{at } x = o \qquad \ldots(19)$$

For the salinity

$$S(z,t)= S_0 \qquad \ldots(20)$$

where; S_0 = the salinity of the river water

1D Flow Model

The system of partial differential equations which describe the 1D incompressible flow in a stream of arbitrary cross section as derived by Saint-Venant in 1871 are;

1- Continuity Equation

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0 \qquad \ldots(1)$$

where; A is the flow cross sectional area (m^2) which is a function of x and t, t is the time (sec), x is the longitudinal distance (m) and Q is the flow rate (m^3/sec).

2- Momentum Equation

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + gA\left(\frac{\partial h}{\partial x} + S_f\right) = 0 \qquad \ldots(2)$$

where; g is the gravity acceleration (m/sec^2), h is the elevation of water surface (m) and S_f is the friction slope which is defined using Manning formula as;

$$S_f = \frac{Q|Q|n^2}{R^{4/3}A^2} \qquad \ldots(3)$$

where R is the hydraulic radius (m) and n is Manning roughness coefficient.

The solution of Eqs, 1 and 2 gives the distribution of h and Q values along the stream. But in order to solve the one dimensional transport equation, the distribution of mean flow velocity (averaged across the cross sectional area of flow), V_x, is required. The values of V_x are obtained as;

$$Vx = Q/A \qquad \ldots(4)$$

Boundary Conditions

For developing 1D flow model, boundary conditions are required to be applied at upstream and downstream ends of the stream.

Upstream boundary conditions

An upstream boundary condition is applied as a flow hydrograph of discharge verses time.

Downstream boundary conditions

Two main types of boundary conditions can be specified at the downstream end of the stream. These boundary conditions include stage hydrograph and flow hydrograph. A stage hydrograph of water surface elevation verses time may be used as the downstream boundary condition if the stream flows into a backwater environment such as an estuary where water surface elevation is governed by tidal fluctuations. A flow hydrograph may be used as the downstream or upstream boundary condition if recorded gage data is available.

Initial Conditions for Flow Model

The specification of initial values needed to solve all the time dependent flow equations is not critical since equilibrium will be established in the model between the driving force and the resultant motion after a certain time (settling down period). Because of that most of previous developed flow models have started with zero water levels and velocities conditions. At the same time, however, the more closely in the initial conditions corresponding with the situation in the field, the less the settling down period.

Determination of Dispersion Coefficient

Dispersion coefficients in 1D and 2D transport equations include the effect of turbulent diffusion and vertical concentration and velocity gradients in 2D plan view model, lateral concentration and velocity gradients in 2D side elevation model or vertical and lateral concentration and velocity gradients in 1D model. Therefore, their values depend mainly on the flow structure within the stream and thus vary spatially and temporally with the changes in flow characteristics.

For 2D plan view model, the values of dispersion coefficients are calculated as;

$$D_x = 63.4n|U|H^{5/6} \qquad \ldots(5)$$

$$D_y = 63.4n|V|H^{5/6} \qquad \ldots(6)$$

where D_x and D_y are dispersion coefficients in x- and y- directions, respectively, (m^2/sec), H is the flow depth (m) and U and V are depth averaged flow velocities in x- and y- directions, respectively, (m/sec).

Eqs. 5 and 6 are based on experimental and theoretical bases. So they need to be corrected if they will be applied to a specific stream. These equations are usually corrected by changing the numeric constants appeared in them during the calibration process of the model.

For 1D transport equation, a general equation for the dispersion coefficient suggested by many researchers has the following form:

$$D = a(Hu_*)(\frac{U}{u_*})^b \left(\frac{w}{H}\right)^c \qquad \text{...(7)}$$

Where;

D= longitudinal dispersion coefficient (m^2/sec).

a, b and c=constants

U= mean flow velocity in x-direction (m/sec)

W= width of stream (m)

H= cross-sectional average flow depth (m).

u_*= bed shear velocity (m/sec).

The bed shear velocity is expressed as;

$$u_* = \sqrt{gRS_f} \qquad \text{…(8)}$$

Where;

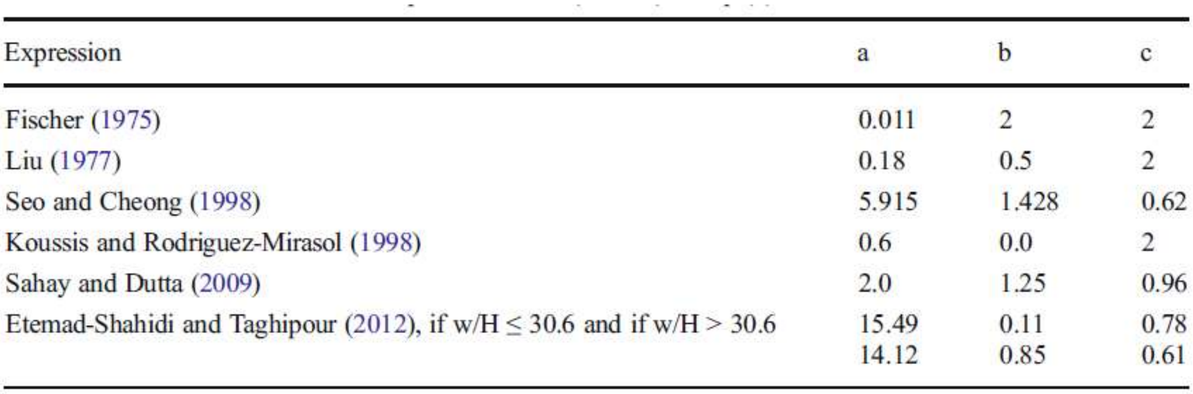
g= gravity acceleration (m/sec^2).

R= hydraulic radius (m).

S_f= gradient of energy line.

The constants of Eq. 7 can be estimated using dimensional and regression analyses from data sets from many rivers over the world. In Table (1), the values of a, b and c suggested by some researchers are presented. *Hint: the reference of Table (1) shall be attached to the lecture.*

Table (1) Constants in the different expressions of D (in m^2/s) in Eq. 7



Expression	a	b	c
Fischer (1975)	0.011	2	2
Liu (1977)	0.18	0.5	2
Seo and Cheong (1998)	5.915	1.428	0.62
Koussis and Rodriguez-Mirasol (1998)	0.6	0.0	2
Sahay and Dutta (2009)	2.0	1.25	0.96
Etemad-Shahidi and Taghipour (2012), if w/H ≤ 30.6 and if w/H > 30.6	15.49 14.12	0.11 0.85	0.78 0.61

The data sets presented in Table 1 are highly varied, thus, it is necessary to derive the suitable data set for specific stream based on hydraulic characteristics of that stream.

Boundary Conditions for Transport Equations

Regardless of model type, 3D, 2D pan view, 2D side elevation or 1D model, the applied boundary conditions are;

At solid boundary, the normal flux is specified to be zero (i.e., there be no dispersive flux of the constituent through the solid boundaries (stream sides and bottom);

For 2D plan view model

$$\frac{\partial c}{\partial n} = K_x \frac{\partial c}{\partial x} l_x + K_y \frac{\partial c}{\partial y} l_y = 0 \qquad \ldots(9)$$

For 2D side elevation model

$$\frac{\partial c}{\partial n} = K_x \frac{\partial c}{\partial x} l_x + K_z \frac{\partial c}{\partial y} l_z = 0 \qquad \ldots(10)$$

At the free surface (2D side elevation model);

Normal flux=0 (Eq.10)

At upstream open boundary;

Constituent concentration is specified to be constant.

At downstream open boundary;

If downstream boundary is subjected to tide fluctuations.;

Constituent concentration is specified to be a function of time.

If downstream boundary is not subjected to tide fluctuations (like the case of inland surface water streams);

Constituent concentration is specified to be constant.

At locations of wastewater disposal (sources of pollution);

The discharge locations of wastewater are treated as point sources. During discretization of stream domain, a node is specified at the location of each point source. If node k represents the discharge location of a specific pollutant, denoted by O, and it is required to simulate the concentration field of pollutant-O, then, the rate of O concentration increase at node k due to external source, L_O, must be defined. The value of L_O can be obtained as;

$$L_O = \frac{Q.EXL_O}{3600V} \qquad \ldots(11)$$

Where;

Q= wastewater flow rate (m^3/hr.).

EXL_O= concentration of pollutant-O in the discharged wastewater (mg/l).

V= volume of water in the initial mixing zone which varies with time due to the variation of water depth at node k (m^3).

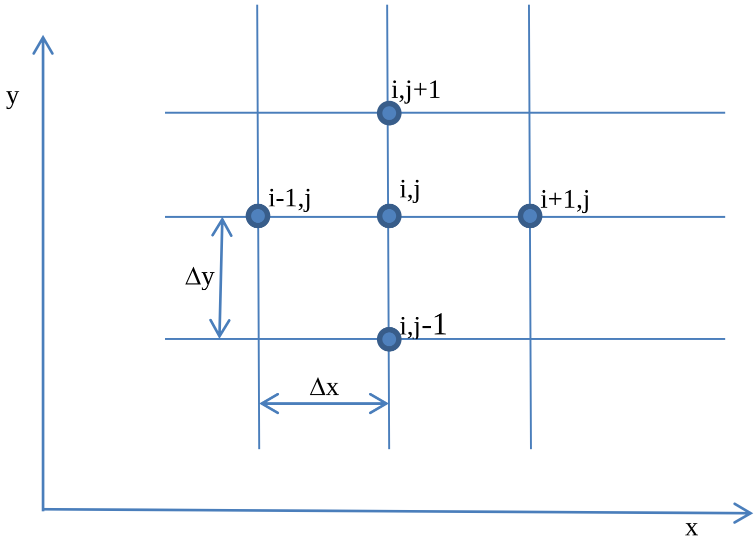
L_O= the rate of O-concentration increase at node k which is assumed to be equal to the rate of O-concentration increase in the initial mixing zone (mg/l/sec).

Solution of Transport Equations Using Finite Difference Method

The partial differential equations governing the flow and transport of different constituents in surface water bodies are solved using numerical methods such as finite element, finite difference, finite volume and boundary element methods. The details of these methods are beyond the scope of this course. However, some simple applications shall be solved using finite difference method (FDM). Outlines on using FDM in solving the transport equation are presented below.

Space Derivatives Representation Using FDM

The finite difference approximation of the space derivatives in the transport equation are;



2D finite difference discretization

1. **Forward difference**;

$$\frac{\partial C}{\partial x} = \frac{C_{i+1,j} - C_{i,j}}{\Delta x} \quad ; \quad \frac{\partial C}{\partial y} = \frac{C_{i,j+1} - C_{i,j}}{\Delta y}$$

2. **Backward difference**;

$$\frac{\partial C}{\partial x} = \frac{C_{i,j} - C_{i-1,j}}{\Delta x} \quad ; \quad \frac{\partial C}{\partial y} = \frac{C_{i,j} - C_{i,j-1}}{\Delta y}$$

3. **Central difference**;

$$\frac{\partial C}{\partial x} = \frac{C_{i+1,j} - C_{i-1,j}}{2\Delta x} \quad ; \quad \frac{\partial C}{\partial y} = \frac{C_{i,j+1} - C_{i,j-1}}{2\Delta y}$$

Time derivatives Representation Using FDM

If the transport equation is written as;

$$\frac{\partial C}{\partial t} = \emptyset(t) \qquad \ldots(12)$$

where ϕ(t) includes all the terms in transport equation excluding the time derivative term, the finite difference approximations of the time derivative term using different finite difference schemes are;

Explicit scheme;

$$\frac{\partial c}{\partial t} = \frac{c_i^{t+\Delta t} - c_i^t}{\Delta t} \quad ; \qquad \emptyset(t)\ is\ evaluated\ at\ time = t$$

Eq.12 can be written as;

$$\frac{c_i^{t+\Delta t} - c_i^t}{\Delta t} = \emptyset(t)^t$$

Implicit scheme;

$$\frac{\partial c}{\partial t} = \frac{c_i^{t+\Delta t} - c_i^t}{\Delta t} \quad ; \qquad \emptyset(t)\ is\ evaluated\ at\ \ time = t + \Delta t$$

Eq.12 can be written as;

$$\frac{c_i^{t+\Delta t} - c_i^t}{\Delta t} = \emptyset(t)^{t+\Delta t}$$

Crank Nicolson (or trapezoidal rule); $\frac{\partial c}{\partial t} = \frac{c_i^{t+\Delta t} - c_i^t}{\Delta t}$; $\emptyset(t)\ \ is\ evaluated\ at\ time = t + \frac{\Delta t}{2}$

Eq.12 can be written as;

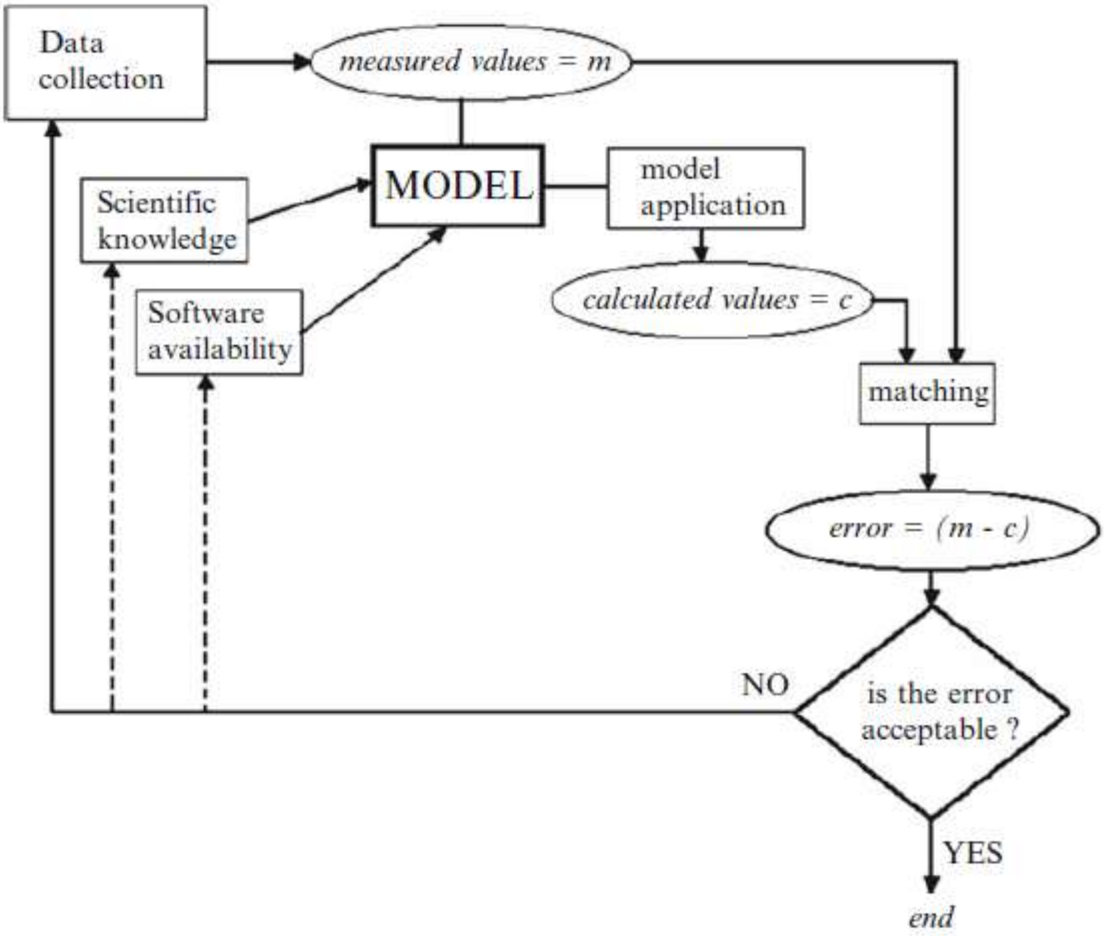
$$\frac{c_i^{t+\Delta t} - c_i^t}{\Delta t} = \frac{1}{2}\left[\emptyset(t)^t + \emptyset(t)^{t+\Delta t}\right]$$

It is important to mention here that the explicit scheme is conditionally stable where convergence condition called Courant Number must be less than 1. Courant number is defined as;

Courant number=$\frac{U.\Delta t}{\Delta x}$

Model Calibration and Verification

Calibration and verification of mathematical models are important steps of models development. During calibration, the model coefficients (constants) are adjusted until the predicted values match an observed data set, see the figure below. The core in the calibration procedure consists of the error, the difference between the calculated and measured values of some significant terms. It has to be stressed that even the measured values may be inaccurate and, therefore, a thorough analysis of the accuracy of the available data is always necessary.



Calibration procedure of the mathematical model

The most immediate way to revise the model is to change the values of the constants and within some pre-established ranges. However, if the error remains unacceptable, it is necessary to revise also some basic assumptions or to check some basic mathematical formulations in the model.

During verification (or validation) process the model is run on another “independent” data set without adjusting model coefficients to see if the model reproduces observed data in the prototype.

Calibration of Flow Model

The most readily available parameters for calibrating hydrodynamic flow model are tidal height at different locations. However, if the purpose of the model is to predict currents for pollutant transport, the calibration against tidal elevation provides little assurance that predicted events are accurate. Consider further that long term pollutant transport is of interest, comparing instantaneous model currents with instantaneous measured currents may not be appropriate. Rather, comparison should be made of long term net currents measured by tracers.

Calibration is done by spatially varying roughness coefficient (Manning or Chezy coefficient) and eddy viscosity coefficients till a good agreement between measured and predicted values is obtained. Before model calibration, it is necessary to perform sensitivity analysis. A sensitivity analysis determines how different values of model inputs affect a particular dependent variable under a given set of assumptions.

Calibration of Water Quality Model

The water quality (or pollutants transport) model must be calibrated so that simulated data for specific constituent are in acceptable agreement with measured ones. The water quality model can be calibrated based on data collected from;

- Synoptic surveys.
- Long-term surveys.
- Special field and laboratory studies.

Model Evaluation Strategy

To evaluate the performance of a developed model, statistical measures are used. These measures include;

1. Standard error of estimate, SE, and its coefficient of variation, CV, measure the precision with which the model tracks observed data variations:

$$SE = \left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{0.5}$$

$$CV = \frac{SE}{\bar{O}}$$

Where; Pi and Oi are the predicted and observed data, respectively, N is number of data points and $\bar{O}$ is the mean of observed data.

2. Linear regression statistics;

$$O_i = aP_i + b$$

The slope, a, measures the accuracy by which model results follow the observed data. The intercept, b, can point out systematic errors in the model. The correlation coefficient, R, measures the precision which the model reproduces observed data trends.