WATER QUALITY MODELLING OF A LAKE

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INTRODUCTION

Lake plays an important role in providing the requirement of water for irrigation, drinking, and industrial use, waste assimilation, and recreation, etc. in many places, in addition to supporting environmental and ecological balance of that area in which a lake dependent activities exist. It is also the source of drinking water for wild and domestic animals and birds, as well as, the shelter place for aquatic lives. Lake water gets polluted by the effluents from municipal, industrial, and agricultural areas, and sometimes due to incidental spills of radioactive tracer from nuclear power plants. Effluents of municipal and industrial sources belong to the point source pollution and the pollution from irrigation return flow belongs to the non-point or diffused source. Since history of our civilization, almost all human activities have grown on banks of water bodies because of the facts that water bodies provide fish as food; and clean water for drinking, bathing, recreation; and irrigation water for development of civilization. The other important aspect of development of human activities on the bank of water bodies is due to ease in disposal of wastewater generate from various human activities into the water bodies at almost no economic cost. Disposal of effluents originating from municipal, industrial, and agricultural sources into water bodies including Lakes is a traditional concept. Lake water has a limiting cleansing capacity of effluents, which depend upon its geometry, flow characteristics and ambient climatic condition etc. Disposal of pollutants more than the self-cleaning capacity of the Lake's water would not only deteriorate the water quality but would also affect the bio-diversity and the ecosystem maintaining by the Lake.

When a solute cloud is injected into a Lake, the Lake water disperses and carries it further to its water volume. As the solute cloud moves, the cloud domain gets lengthened, the sharp variation in concentration at interface of solute and medium flattens, the peak concentration reduces and the solute gets distributed in the ever-increasing volume of water. These physical consequences are result of flow and mixing mechanisms, known as advection, diffusion and dispersion. Diffusion and dispersion combined is known as hydrodynamic dispersion. Advection is the bodily movement of a parcel of fluid resulting from an imposed current, where as diffusion is the scattering of particles by random or turbulent motion in microscopic scale, and dispersion is the scattering of particles or cloud of contaminants by the interaction of differential advection and cross-sectional diffusion in a greater scale. Diffusion is a component of dispersion. When water is stagnant, only diffusion process takes place.

When confronted with water pollution problem, the people responsible for its solution will ask several questions:

(1) what is the nature of the pollution:
- *is it miscible or not to the water ?*
- *what are its physical and chemical properties ?*
- *what sort of danger does it present ?*

(2) What is the scale of pollution:
- *what is the total amount of pollution ?*
- *what is the strength of the pollution source ?*
- *what are the dimensions and the geometrical characteristics of the pollution source ?*
- *what is the duration of the pollution ?*

Answers to these questions are necessary to formulate the problem and to develop predictive model. A model is a conceptualization of reality that is represented by mathematical equations, which are interpreted to get the insight of the problems.

TRANSPORT MECHANISM

There are many processes, which govern the transport mechanism in a Lake water system. These processes may be either physical, chemical biological or combination of them. The principal processes, which are predominant and most often used by the modelers, are advection, diffusion and dispersion, adsorption, biodegradation, sources and sinks, and radioactive decay. Let us define the terms used in transport mechanism.

Advection: is the bodily movement of contaminants along with flowing water at the advective flow velocity.
Diffusion: on account of molecular mass transport process by which the solutes move from areas of higher concentration to areas of lower concentration.
Dispersion: on account of mixing process due to variation of velocity in flowing media.
Adsorption: process of sorption, interaction of contaminant with solid, partitioning of organic contaminants from soluble phase into the solid matrix.
Bio-degradation: transformation of certain organic species to simple CO_2 and water in the presence of microbes in the subsurface.
Sources and sinks: the solute may enter into or leave from the water body through sources or sinks. Discrete and distributed pollutant sources are examples of solute sources and sinks.
Radioactive decay: the radioactive components within the fluid decreases the concentration as a result of decay over time.

The principal characteristics of Lakes that are of interest include: Geometry, (width and depth), slope, Velocity, Flow, Mixing characteristics, Lake water temperature, Suspended solids, sediment transport, etc.

For Lake water quality management, the important chemical characteristics are: DO variations including associated effects of oxidizable nitrogen on the DO regime; pH, acidity, alkalinity relationships in areas subjected to such discharges; Lake water temperature, Total Dissolved Solids(TDS) and chlorides; Chemicals that are potentially toxic, etc.

Significant Biological characteristics, which are important in water quality studies, are:

Bacteria and Viruses, Fish populations, Rooted aquatic plants, and Biological slimes.

NATURE OF INPUTS

The principal inputs in a Lake can broadly be divided into two categories: (a) point sources, and non-point sources. The point sources are those inputs that are considered to have a well-defined point of discharge. Municipal discharges and Industrial discharges are two principal point sources. The principal non-point sources are: (a) agricultural, (b) silviculture, (c) atmospheric, (d) urban and suburban runoff, and (e) groundwater.

GOVERNING EQUATIONS

The basic principle of Lake water quality modeling is the conservation of mass. The governing equation describing the advection-dispersion, sources and sinks terms for steady and uniform flow condition in a three-dimensional lake system can be expressed as:

$$\frac{\partial C_i}{\partial t} = -\frac{\partial (UC_i)}{\partial x} - \frac{\partial (VC_i)}{\partial y} - \frac{\partial (WC_i)}{\partial z} + \frac{\partial}{\partial x}\left(D_x \frac{\partial C_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_i}{\partial z}\right) \pm \sum S_i \quad \text{............(1)}$$

where C_i= concentration of the i[th] water quality constituent, (ML^{-3}); U, V, and W = the water velocity components in longitudinal (x), lateral (y), and vertical (z) directions (LT^{-1}); t = time coordinate, (T) ; D_x, Dy and Dz = the diffusion coefficients in x, y, and z direction respectively ($L^2 T^{-1}$); $\sum S_i$ = the effective source/sink terms, which include the kinetic transformation rate, external loads and sinks for the i[th] water quality constituent ($ML^{-3}T^{-1}$).

The concentration, C_i represents water quality constituent of interest, whose fate is to be determined on both time and space. In the above eq.(1), having known U, V, and W and, D_x, Dy and Dz; the ; the fate of any water quality constituent, C_i both on time and space can be computed for known quantity of source or sink, $\sum S_i$ in the system, whose water quality fate is to be simulated.

Eq. (1) represents a 3-dimensional partial differential equation (PDE) whose straight forward analytical solution is difficult rather not available for complex hydraulic conditions. However, Eq.(1) can be solved approximately using numerical schemes such as; finite difference scheme, finite element scheme, etc. There are numbers of source codes available derived based on the Eq. (1), which can be straightway be applied to successfully model or simulate water quality constituents of interest for a lake; these models are : WASP5 & 6; HYDRODYNAMIC MODEL; CE-QUAL-W2, MODFLOW LAKE PACKAGE, etc.

FACTORS AFFECTING LAKE WATER QUALITY

The nutrient status of lakes is strongly related to their depth and the types of land use and human activities in the catchment. Deep lakes have a greater capacity to absorb incoming nutrients before showing definite signs of deterioration in water quality. The monitored lakes that have high levels of nutrients tend to be shallow. The monitored lakes with the lowest levels of nutrients are nearly all deep lakes and do not have particularly intensive farming or urban activity in their catchments.

Levels of nutrients (nitrogen and phosphorus) and algae tend to be higher in lakes in pastoral catchments than in lakes in natural catchments.
Because algal concentrations affect water clarity, the lakes in natural catchments have water that is clearer than water in lakes in pastoral catchments.

Natural factors such as air temperature and wind are also important determinants of water quality in lakes. Algal blooms are more likely to occur in lakes in warmer climates (those at lower elevations and in the north) and in the summer. Wind can create waves and currents, particularly in shallow lakes, which lift sediments from the lake bed into the water. As well as reducing the clarity of water, this can increase the amount of nutrients available for algal growth. Clarity and the appearance of lake water may be affected by soil type. For example, lakes surrounded by peaty soil have water that is naturally brown-stained or 'dirty' looking.

EUTROPHICATION OF LAKE

Eutrophy means a state of good nutrition. Plants require a number of nutrients, but to vastly different degrees. Some nutrients, such as carbon, nitrogen, potassium, and phosphorous are needed in large quantity. These are termed macronutrients. Since nitrogen and phosphorous are commonly in limited supply, many impoundments tend inherently to be clear and essentially free of clogging algae and vascular plants. Over long period of time and depending on geological conditions, natural sources of nutrients may lead to eutrophication in lakes.

Eutrophication is the process of increasing nutrients in surface waters. The presence of nutrients in an impoundment generally favors plant growth. Depending upon antecedent conditions, the relative abundance of nitrogen, phosphorous, light, and head, and the status of a number of other physical and chemical variables, the predominant forms may be diatoms, other microscopic or macroscopic algae, or bottom-rooted or free-floating macrophytes.

LAKE ECOSYSTEM MODELING

The concept of a lake's health is somewhat easy to relate to humans, because they have an idea of what is healthy and well-functioning for humans and what is not. Nevertheless, defining a lake's health in the scientific world is not as clear, and is a subject of debate. One suggested concept of lake health includes a range of biological, physical, and aesthetic parameters as well as management, policy, and "value" considerations. To achieve such a complex conception of a lake's health, a multidisciplinary approach is required.
Moreover, a combination of methods is needed because a single indicator of lake health is inadequate. Some of these methods measure ecosystem functions (e.g., primary productivity and nutrient cycling); ecosystem structure (e.g., diversity and abundance); internal processes (e.g., water circulation, residence time, temperature, and light); and external inputs (e.g., nutrients, sediment and chemical loads, and rain events).

A lake ecosystem comprises communities of organisms that interact with each other and with the environment that sustains them. These interactions may, in turn, produce changes in the same communities and environment. In a healthy lake, the interactions are necessary to assure the lake ecosystem's sustainability. In an unhealthy ecosystem, the sustainability of the lake's communities is compromised, and in need of human actions to recover it and protect it for future generations.

The balanced coupling of two functions—production and decomposition—is essential for the equilibrium and sustainability of a lake ecosystem. Hence, these ecosystem functions are basic for detecting lake health problems. Primary productivity, or the growth of phytoplankton (predominantly algae), is the main and most basic food source in most lakes. Phytoplankton growth requires that inorganic nutrients (particularly phosphorus and nitrogen), light, and temperature be adequate to meet the primary producers' needs.

Nutrient cycling is the process that recycles, through decomposition, what has not been used or has been discarded by lake organisms. The bacterial community "cleans up" and provides essential nutrients (mainly phosphorus and nitrogen) for the phytoplankton. For this process, most bacteria require oxygen. Over productive lakes will produce excess food that will eventually lead to high rates of decomposition with a consequent high use of oxygen. These conditions contribute to premature lake aging and the likely disappearance of species that are oxygen-sensitive and that require less eutrophic conditions. A schematic representation of the lake ecosystem is given in Figure 1.

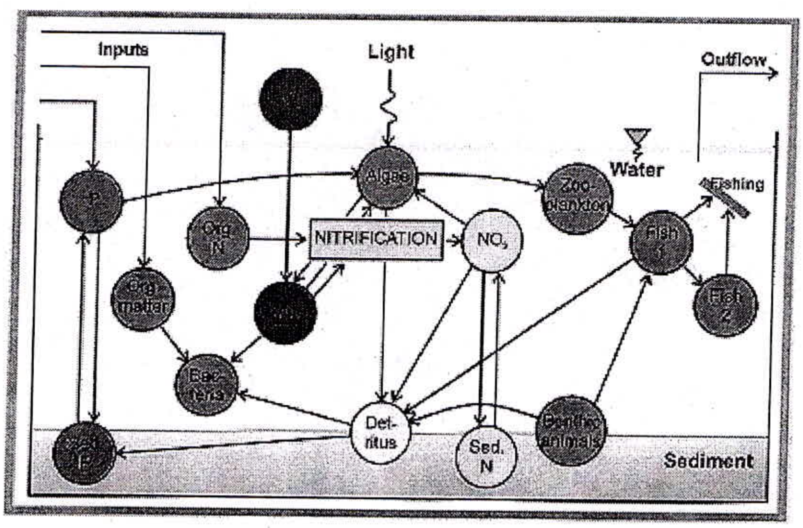

Figure 1. : A schematic representation of ecosystem processes of a Lake

From Fig. (1), it can be seen that the inputs to a Lake are organic matters comprising Phosphorous (P) and organic Nitrogen (N). The organic matters give birth to bacteria as food to them, and the organic Nitrogen takes part in the Nitrification process with the help of atmospheric oxygen and algae. The algal growth takes place with the help of light using some parts of Phosphorous and NO_3, and oxygen. Some parts of Phosphorous get deposited in the Lakebed in the form of sediments. NO_3 that generates from the Nitrification process and consumed by algae some fraction also get deposited in the Lakebed as detritus and with the sediment. The detritus is consumed by benthic animals, and the benthic animals act as food to fish. The zone in which algal growth takes place is called zooplankton, which acts as source of food to fish. The algal growth is governed by the rate at which organic matters, Phosphorous and organic Nitrogen available in a Lake. The Phosphorous and Nitrogen are thus considered as the governing constituents for algal growth in a Lake and these constituents are considered as the limiting factors for Lake Ecosystem balance. For N/P ratios greater than 7.2, phosphorous would be less available for growth (limiting) and when less than 7.2, nitrogen would be limiting. In practice, values of less than 5 are considered nitrogen limiting, greater than 10 are phosphorous limiting, and between 5 and 10, both are limiting. In many cases of eutrophic lakes, nitrogen is not limiting because of the process of nitrogen fixation.

PHOSPHOROUS MODELLING OF A LAKE

If we intended to model the time varying Phosphorous in Lake's water, the following mathematical expressions can hold goods. Let us consider the following block diagram (Fig. 2) in which P_i is the input rate of Phosphorous concentration in the lake; P_L is the Phosphorous in the lake water column; Q_i is the inflow rate of water in the lake; V is the volume of lake; A is the spread area of the lake; and Z is the mean depth of water in the lake.

Mean depth, Z = V/A; hydraulic flushing or dilution rate = Q/V; hydraulic loading, q = Q/A; Mass of loading = $Q_i P_i$, where Q is the outflow rate from the lake.

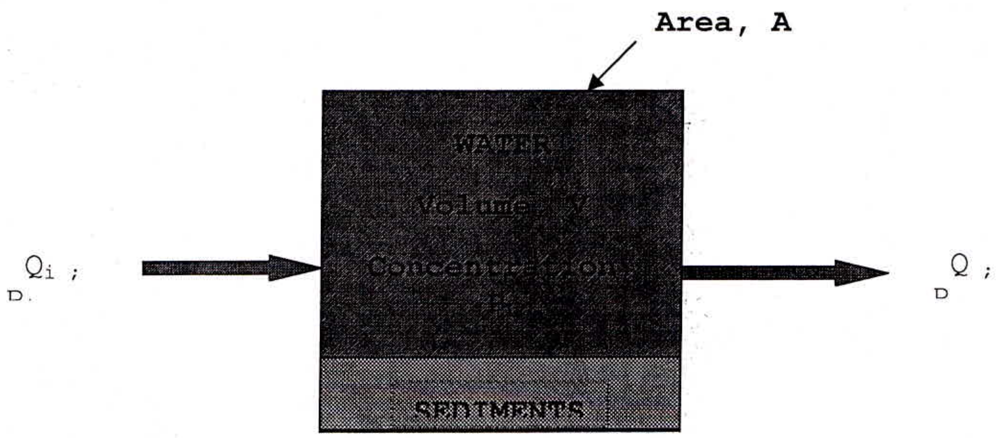

Figure 2 : Block diagram of mass balance of Phosphorous in a Lake

Performing mass balance with the assumption that that lake water is completely mixed and flow is in a steady state condition, i.e., $Q_i = Q$ and annual average rates are constant; we obtain

$$\frac{dP_L}{dt} = \frac{Q\,P_i}{V} - \frac{Q\,P_L}{V} - K\,P_L \qquad \text{........(2)}$$

In which, K is the net rate of solid phase removal and release, proportional to P_L.

Solving for P_L; we get,

$$P_L = \frac{D\,P_i}{D+K} \quad \text{(Mass Balance Form)} \qquad \text{.......... (3)}$$

$$P_L = \frac{M}{Q}\left(\frac{D}{D+K}\right) \quad \text{(Mass Inflow Form)} \qquad \text{.......... (4)}$$

$$P_L = \frac{1}{A\,Z}\left(\frac{M}{D+K}\right) \quad \text{(Loading Form)} \qquad \text{.......... (5)}$$

D, Z, M, and A are as explained earlier.

Any of three different forms of the steady state equation as given by Eqs (3) – (5) can be used to predict phosphorous concentration in lakes. Each form may be more or less suitable for a specific data set. The important variables are the hydraulic flushing or dilution rate, Q/V which is inverse of residence time; lake volume to area ratio, V/A; influent phosphorous concentration, P_i; and the net rate of removal, K.

The variables Q, V, A are to be determined from other data. The influent Phosphorous concentration, P_i can be based on measurements or estimated from calculations. Estimation of the net removal rate, K is not as clear. Vollenweider (1976) and Larsen and Mercier (1976) independently estimated the net rate of removal as a function of dilution rate:

$$K = \sqrt{D} \qquad \text{......... (6)}$$

This is the most accepted approach for screening the value of K. Jones & Bachmann (1976) estimated that K = 0.65 by least squares fitting of data for 143 lakes.

Also 'K' can be estimated from the ratio of the measured mass phosphorous retained and the mass inflow:

$$R = \frac{Q_i\,P_i - Q\,P_L}{Q_i\,P_i} \cong \frac{P_i - P_L}{P_i} \qquad \text{.......... (7)}$$

and, $$K = \frac{M\,R}{A.\,Z.\,P_L} \qquad \text{.......... (8)}$$

Vollenweider and Kerekes (1981) based on the analysis of results classified lakes into discrete groups according to their eutrophication characteristics as given below in Table-1.

Table 1. Preliminary Classification of Trophic State of Lake
(Vollenweider and Kerekes,1981)

Variable*	Oligotrophic	Mesotrophic	Eutrophic
Total Phosphorous			
Mean	8	27	84
Range	3 - 18	11 - 96	16 - 390
Total Nitrogen			
Mean	660	750	1900
Range	310 - 1600	360 - 1400	390 - 6100
Chlorophyll a			
Mean	1.7	4.7	14
Range	0.3 – 4.5	3 - 11	2.7 - 78
Peak Chlorophyll a			
Mean	4.2	16	43
Range	1.3 - 11	5 - 50	10 - 280
Secchi Depth, m			
Mean	9.9	4.2	2.4
Range	5.4 - 28	1.5 – 8.1	0.8 – 7.0

* µg/l (or mg/m^3)except Secchi depth.

FRAMEWORK OF A MODEL

Principal components of modeling framework are schematically shown in Fig. 3.

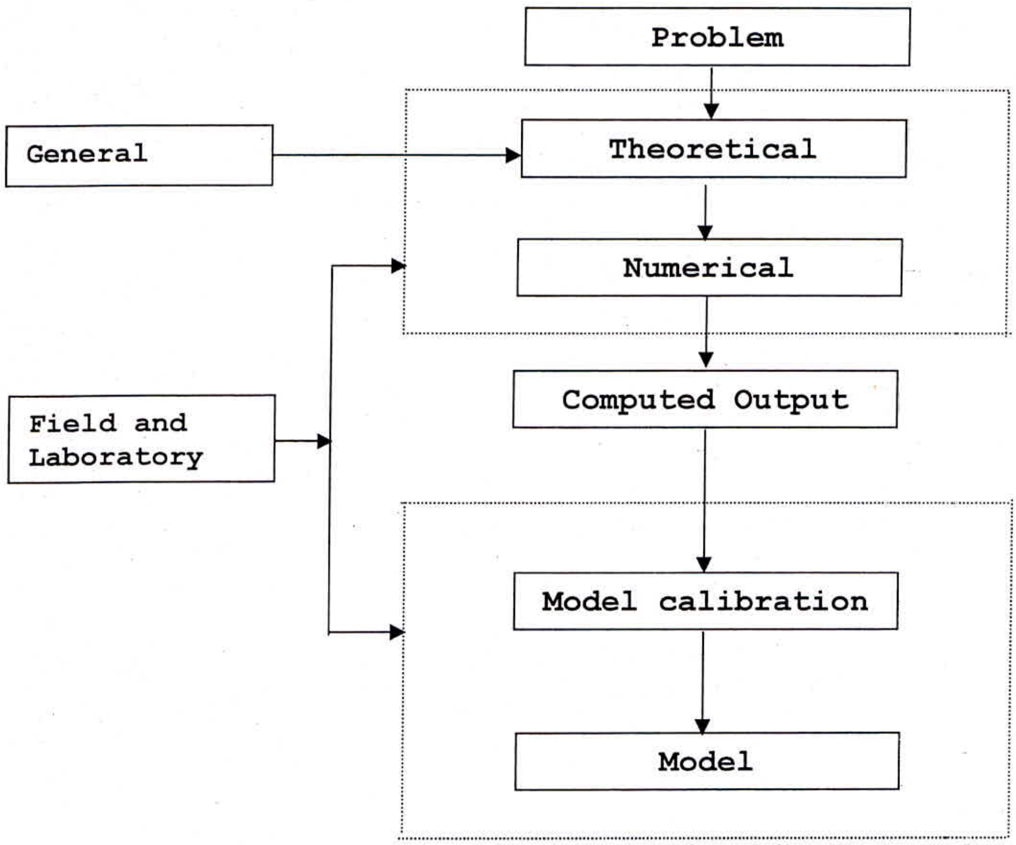

Figure 3. Principal Components of Modeling Framework

NUMERICAL METHOD IN WATER QIALITY MODELING

Based on the intended objectives and nature of the study, different concepts can be applied to formulate a model particularly for solving the real-life situations confronted with a number of options. The effectiveness of the outputs of the model depends on how accurately one conceptualizes the problem, and strength of the input database. For a one-dimensional straightforward simple boundary condition problem, an analytical model can give solutions. However, for problems of complex boundaries and varying hydrological conditions, which is usually observed in most of the real-life situations, analytical solutions of the equation of flow and contaminant transport are not available. The method suitable for solving a real-life flow and transport problem is the numerical modeling due to its capability in solving large and complex water quality problems having spatial heterogeneity.

In numerical solution, Finite difference Method (FDM) is one of the most popular schemes to solve the partial differential equations (PDE). FDM includes three major steps. First, a grid, and the time interval into time steps divide the flow region. Second, the partial derivatives involved in the PDE are replaced by their finite difference approximations. As a result, the PDE is transformed into a system of algebraic equations. Third, the algebraic system is solved and the nodal values of the unknown functions are obtained. These discrete values approximately describe the time-space distribution of the unknown variable. Let us see, how the above steps are used to solve the advection-dispersion problem for one-dimensional case, which can be obtained from Eq. (1) by considering y and z-directional components as zero.

Consider that there are three adjacent nodes along the x-direction, (x-Δx, y,z), (x,y,z), and (x+Δx, y,z) in the center of each cube, as shown in Fig.4. Denoting the nodes number as (i-1, j, k),(i, j, k), and (i+1, j, k), and the spatial distances between the mesh planes as Δx, Δy, and Δz.

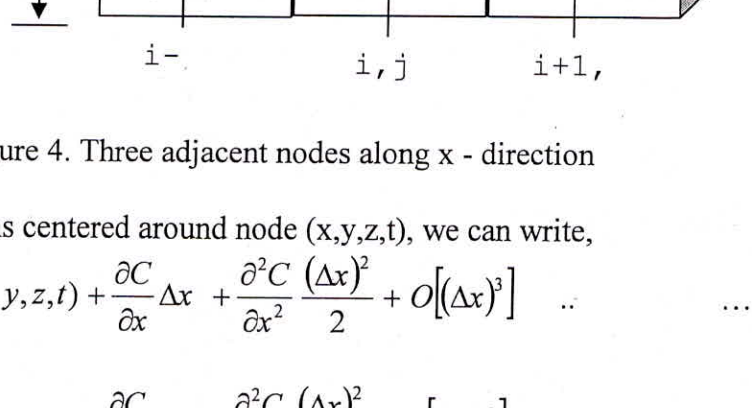

Figure 4. Three adjacent nodes along x - direction

Using Taylor expansions centered around node (x,y,z,t), we can write,

$$C(x+\Delta x, y, z, t) = C(x, y, z, t) + \frac{\partial C}{\partial x}\Delta x + \frac{\partial^2 C}{\partial x^2}\frac{(\Delta x)^2}{2} + O\left[(\Delta x)^3\right] \quad \text{........ (9)}$$

and

$$C(x-\Delta x, y, z, t) = C(x, y, z, t) - \frac{\partial C}{\partial x}\Delta x + \frac{\partial^2 C}{\partial x^2}\frac{(\Delta x)^2}{2} + O\left[(\Delta x)^3\right] \quad \text{........ (10)}$$

From Eq.(9) , we have

$$\frac{\partial C}{\partial x} = \frac{C(x+\Delta x, y, z, t) - C(x, y, z, t)}{\Delta x} + O(\Delta x) \qquad \text{........... (11)}$$

From Eq.10,

$$\frac{\partial C}{\partial x} = \frac{C(x, y, z, t) - C(x-\Delta x, y, z, t)}{\Delta x} + O(\Delta x) \qquad \text{........... (12)}$$

Subtracting Eq. 10 from Eq.9,

$$\frac{\partial C}{\partial x} = \frac{C(x+\Delta x, y, z, t) - C(x-\Delta x, y, z, t)}{2\,\Delta x} + O\left[(\Delta x)^2\right] \qquad \text{............ (13)}$$

By neglecting the second term on the right-hand side of Eqs. 11, 12, & 13, three approximate equations are obtained. These three equations are called the *forward, backward, and central difference formulas* respectively. The second term on the right-hand side is called the truncation error.

The summation of Eqs.9 and 10, generates the finite difference approximation of the second order derivative:

$$\frac{\partial^2 C}{\partial x^2} = \frac{C(x+\Delta x, y, z, t) - 2C(x, y, z, t) + C(x-\Delta x, y, z, t)}{(\Delta x)^2} \qquad \text{.......... (14)}$$

The truncation error of this approximation is $O\left[(\Delta x)^2\right]$. For node numbers, replace x, y and z by i, j, and k respectively.

Finite Difference Solutions for 1-D ADE

The 1-Dimensional advection-dispersion equation (ADE) Eq.(1) with V, W, D_y, D_z, and S_i = 0 is given by:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x}; \qquad 0 \le x \le L; \quad 0 \le t \le T \qquad \text{.......... (15)}$$

The time range (0, T) and space region (0,L) are both divided into a uniform grid with time and space intervals Δt, and Δx, respectively. The concentration value of the i-th node located at x_I, and at time t_n, may be written as $C_{i,\,n}$. Now let us derive a finite difference equation at any interval node to replace Eq.15. The L.H.S. of Eq. 15 is approximated by forward difference:

$$\frac{\partial C}{\partial t} = \frac{C_{i,n+1} - C_{i,n}}{\Delta t} \qquad \text{.......... (16)}$$

On the R.H.S. of Eq.15, $\partial^2 C / \partial x^2$ is replaced by Eq.14 and $\partial C / \partial x$ may be replaced by forward, backward, or central formula, Eq.11, Eq.12, and Eq.13. If t in Eq. 13 and 12 are replaced by t_n, t_{n+1}, or the middle time between t_n, t_{n+1}, three finite difference schemes can be obtained, that is, the explicit, implicit, and Crank-Nicolson schemes.

The explicit difference equation of Eq.15 is:

$$\frac{C_{i,n+1}-C_{i,n}}{\Delta t} = D_L \frac{C_{i+1,n}-2C_{i,n}+C_{i-1,n}}{(\Delta x)^2} - U\frac{C_{i+1,n}-C_{i-1,n}}{2\Delta x} \quad \text{.......... (17)}$$

From this equation, we can directly obtain,

$$C_{i,n+1} = \left[\frac{D_L\,\Delta t}{(\Delta x)^2}+\frac{U\,\Delta t}{2\Delta x}\right]C_{i-1,n} + \left[1-\frac{2D_L\,\Delta t}{(\Delta x)^2}\right]C_{i,n} + \left[\frac{D_L\,\Delta t}{(\Delta x)^2}-\frac{U\,\Delta t}{2\Delta x}\right]C_{i+1,n} \quad \text{.......... (18)}$$

Therefore, the concentration values of all nodes at time t_{n+1} can be calculated directly without solving any equations, provided that their values at t_n are known.

The implicit difference equation of Eq.15 is:

$$\frac{C_{i,n+1}-C_{i,n}}{\Delta t} = D_L \frac{C_{i+1,n+1}-2C_{i,n+1}+C_{i-1,n+1}}{(\Delta x)^2} - U\frac{C_{i+1,n+1}-C_{i-1,n+1}}{2\Delta x} \quad \text{.......... (19)}$$

where the unknown concentrations $C_{i-1,\,n+1}$, $C_{i,\,n+1}$, and $C_{i+1,\,n+1}$ at t_{n+1} are included. After rearrangement, we have

$$C_{i,n} = -\left[\frac{D_L\,\Delta t}{(\Delta x)^2}+\frac{U\Delta t}{2\Delta x}\right]C_{i-1,n+1} + \left[1-\frac{2D_L\,\Delta t}{(\Delta x)^2}\right]C_{i,n+1} - \left[\frac{D_L\,\Delta t}{(\Delta x)^2}-\frac{U\,\Delta t}{2\Delta x}\right]C_{i+1,n+1} \quad \text{...... (20)}$$

We can write similar equations for all nodes. When these equations are combined with boundary conditions, a set of tridiagonal equations is formed. Thus, the concentration values of all nodes can be obtained by using the Thomas algorithm.

The Crank-Nicolson difference scheme:

The explicit and implicit schemes can be averaged to yield the Crank-Nicolson difference scheme:

$$\frac{C_{i,n+1}-C_{i,n}}{\Delta t} = \frac{1}{2}\left(D_L \frac{C_{i+1,n}-2C_{i,n}+C_{i-1,n}}{(\Delta x)^2} - U\frac{C_{i+1,n}-C_{i-1,n}}{2\Delta x} + D_L \frac{C_{i+1,n+1}-2C_{i,n+1}+C_{i-1,n+1}}{(\Delta x)^2} - U\frac{C_{i+1,n+1}-C_{i-1,n+1}}{2\Delta x}\right) \quad \text{.......... (21)}$$

After rearranging,

$$-\left[\frac{D_L\Delta t}{(\Delta x)^2}+\frac{U\Delta t}{2\Delta x}\right]C_{i-1,n+1} + 2\left[1-\frac{D_L\Delta t}{(\Delta x)^2}\right]C_{i,n+1} - \left[\frac{D_L\Delta t}{(\Delta x)^2}-\frac{U\Delta t}{2\Delta x}\right]C_{i+1,n+1}$$
$$= \left[\frac{D_L\Delta t}{(\Delta x)^2}+\frac{U\Delta t}{2\Delta x}\right]C_{i-1,n} + 2\left[1-\frac{2D_L\Delta t}{(\Delta x)^2}\right]C_{i,n} + \left[\frac{D_L\Delta t}{(\Delta x)^2}-\frac{U\,\Delta t}{2\Delta x}\right]C_{i+1,n} \quad \text{.......... (22)}$$

The R.H.S of Eq.22 includes only the known concentrations at t_n. Using Thomas algorithm we can solve tridiagonal equation to obtain concentration values at t_{n+1}.

For explicit scheme, the restrictive condition would be:

$$\Delta t < \frac{(\Delta x)^2}{(2D+V\Delta x)} \quad \text{......... (23)}$$

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