CHAPTER 5

SURFACE WATER QUALITY MODELING

5.1 Introduction

5.1.1 General

Both natural processes and human activities influence the quality of surface waters. The natural processes and their sources of pollution in surface water bodies are relatively inconsequential, except pollution from natural disaster. Surface water pollution and contamination from humans and human activities, comprising both organic and inorganic constituents, known as anthropogenic pollutants, originate from domestic and municipal source, agricultural production, mining, industrial production, power generation, forestry practices, and other factors, which alter the physical, chemical and biological characteristics of water, are of main concern for surface water bodies. Amongst these sources, the major pollution is from human settlements, industrial and agricultural activities. Pollution and contamination from such sources manifest itself in the form of higher concentration of nutrients, sediments, salts, trace metals, chemicals and other toxins, as well as pathogenic organisms that may thrive in warmer and contaminated waters. In addition, a growing number of new contaminants are being detected in the world's waterways (UN-Water, 2011). These include contaminants from pharmaceutical products, steroids and hormones, industrial additives and agents, as well as gasoline additives (WHO, 2011; UL, 2015; Eslamian, 2016). These contaminants present a new challenge to water quality management (UN-Water, 2011). The synergistic interactions of these contaminants and pollutants may result in complex concoctions that are difficult to treat.

Degraded surface water quality affects the aquatic environment. The degradation of ecosystem affects people most who live near the contaminated waterways and those who have no alternate access to safe water or improved sanitation. Although the "water crisis" tends to be viewed as a water quantity problem, water quality is increasingly recognized in many countries as a major factor in the water crisis (UN-Water, 2011). Historically, poor water quality has been principally associated with public health concerns through transmission of water-borne diseases.

Declining water quality is a global issue of concern as human populations grow, industrial and agricultural activities expand, and climate change threatens to cause major alterations to the hydrological cycle (UN-Water, 2011). Globally, the most prevalent water quality problem is eutrophication particularly in lentic water bodies, a result of high-nutrient loads (mainly phosphorus and nitrogen), which substantially impairs beneficial uses of water. Major nutrient sources include agricultural runoff, domestic sewage (also a source of microbial pollution), industrial effluents and atmospheric inputs from fossil fuel burning and bush fires. Lakes and reservoirs are particularly susceptible to the negative impacts of eutrophication because of their complex dynamics, relatively longer water residence times and their role as an integrating sink for pollutants from drainage basins (Zhen-Gang, 2008).

5.1.2 India's status of river water quality

India has a large network of rivers across its length and breadth. It has also huge numbers of surface water bodies, viz. lakes, reservoirs, tanks, ponds, etc, of varying sizes spread over the country. Those surface water bodies in many parts of the country act as the sources of drinking and agricultural water in addition to the eco-system services of the area. Unfortunately, the nation is unable to retain these rich natural resources of surface water bodies including rivers, because of deteriorating water quality. Water pollution is a major environmental issue in India and its concern is mainly because of discharge of untreated sewage in water bodies. The reports of Central Pollution Control Board (CPCB, 2011; 2013) estimate that 75-80% of water pollution by volume is due to organic pollution measured in terms of bio-chemical oxygen demand (BOD) and coliform bacterial count. As reported, it was mainly due to discharge of untreated domestic wastewater from the urban centres of the country. The municipal bodies at large are not able to treat increasing load of municipal sewage flowing into water bodies. On the other hand, the receiving water bodies also do not have adequate water for dilution because of abstraction structures and diversion of water from the river. Further, there is a large gap between generation and treatment of domestic wastewater in India (CPCB, 2011; 2013). The problem is not only that India lacks sufficient treatment capacity but also that the sewage treatment plants that exist do not operate and maintain properly. The report (CPCB, 2009) showed that out of estimated 38,354 million litres per day (MLD) of sewage generation from major cities of India; only 30.8% is treated and remaining untreated sewages flow on/in to overland, rivers/streams and other surface water bodies. The situation of treatment of industrial wastewater is somewhat better, out of 13,468 MLD generates from about 57,000 major polluting industries, 60% is treated. Water pollution from diffuse sources viz. agricultural activities, due to application of pesticides and herbicides to control pests, and runoffs of nitrogen (N) and phosphorus (P) applied to agricultural land move with rainfall may cause eutrophication to surface water bodies. Municipal sewages along with agricultural run-offs and industrial effluents are main concern of India's surface water pollution causing deteriorated water quality including eutrophication.

5.1.3 Issues related to lakes and estuaries

The word "Lake" is used loosely in India to describe different types of surface water bodies, except rivers/streams. These water bodies are natural, manmade, ephemeral and wetlands. The manmade (artificial) water bodies are generally called reservoirs, ponds and tanks. Ponds and tanks are small in size compared to lakes and reservoirs. Numerous natural lakes of varying sizes are present in India either at high altitude Himalayan region or in low altitude region. Many of the lakes in Himalaya have fresh water with or without inflow and outflow. These lakes have varying chemistry in terms of solutes, bio-geochemistry, mineralogy vis-a-vis eco-hydrology of the water body, which are primarily related to enormous altitude variation governing climate, vegetation, agriculture, lithology, tectonics and intensity of erosion/weathering at source. The high altitude lakes are mostly oligotrophic and are fed from snow-melt, precipitation and spring, whereas lakes of low altitudes receive water from local rains, through streams, *nalas* and spring and some of them have approached a higher level trophic state (eutrophic or hyper-eutrophic) due to strong impact of anthropogenic influence such as tourist influx, unplanned settlements, landuse, development activities in the catchment area, and disposal of municipal and domestic wastes. In general, the Indian lakes have either fresh water or salt water. Some of them are sacred lakes.

Due to alteration of landscapes by denuding forests, urbanization and discharge of wastes, sedimentation and eutrophication have increased in most of Indian lakes. Many high altitude lakes, particularly in Kashmir and Garhwal Himalayans, which remained clean and non-eutrophied for centuries, are showing signs of deterioration. The famous Dal Lake of Kashmir, which was about 40 km^2 of area in the beginning of nineteenth century, has presently about 20 km^2.Almost half of the lake Renuka (Water spread area of 670 ha), the biggest lake of Himachal Pradesh in the lesser altitude of Siwaliks of Himalayan region, is filled up by sediment. The situation is much worst in the plains or in peninsular India. Osmansagar in Hyderabad, Upper Lake in Bhopal and Poondi, Red Hills in Chennai, which are sources of drinking water in the respective area, have shrunk considerably in the recent past causing great hardship to the city dwellers. Due to mismanagement and various other reasons, most of the lakes of smaller sizes located in the urban areas are used as dumping spot of wastes, both solid and liquid. These have resulted in problem of eutrophication. Very precisely, occurrence of inorganic nutrients in water and the resulting increase in plant productivity has led to a serious water quality problem for many lakes in India.

Along the coast line of India, numerous bays and gulfs are formed where big or small rivers meet, thereby forming estuarine zone. Along coastal line numerous brackish water lakes are in existence, which join with sea during floods. A typical Indian estuary is highly productive, as waters receive abundant qualities of nutrients from the connected fresh water systems and surrounding land areas. Most of the Indian estuaries are monsoon dominated. The abundant fresh water influx received by these estuaries is more or less limited to the monsoon season extending from July to October. In the summer months of March to June very little fresh waters are added and the severity of pollution hazards comes into prominence during this period.

The major estuarine systems in India are: Hooghly-Metlah estuarine system, Mahanadi estuarine system, Krishna estuary, Pulicat Lake, Cauvery estuary, Vembanad Lake and Narmada-Tapti estuary. In Mahanadi estuary, the tidal effect is felt only up to about 35 kms upstream of the mouth. In the Gautami, which is the main component of the Godavari estuarine system, the tidal inflow extends up to about 50 km from the mouth. Increase in salinity has been observed in the rivers in recent years.

5.1.4 Water quality challenges in India

Indian rivers and other surface water bodies are primarily monsoon driven except the rivers of Himalayan origin, which carry snow and glacier melt waters during non-monsoon months. India's climate is dominated by temperate and tropical condition. The physicochemical and biological characteristics of domestic and municipal uses of water do not contain any hard lining chemical constituents. Surface water quality problems face by the country have the constituents' characteristics comprising suspended solids, BOD, low DO, Total and Fecal coliform, nutrient loads, etc., which represent contaminants of pathogenic in nature, originate mainly from municipal, agricultural and industrial sources. India has characteristic religious notions of disposal of worships refusals into water bodies. Although, India has a Water Prevention and Control of Pollution Act (1974), its effective enforcement would require a number of political and administrative pursuits. On the other hand, the water quality problems in India are emerging as a major hurdle to attain water security.

Pathogenic (organic) wastes/pollutants discharged into natural water bodies such as; rivers, lakes and the seas disappear slowly with time by the processes called self purification of natural water systems (White and Lack, 1982). The self purification is a complex process that often involves physical, chemical and biological processes working simultaneously. The amount of Dissolved Oxygen (DO) in water is one of the most commonly used indicators of river health. The major physical processes involved in self-purification of a river are dilution, sedimentation and re-suspension, filtration, gas transfer and heat transfer. Lakes and reservoirs are typically standing waters, the former naturally occur and the latter man-made. They exhibit a vast range of surface areas, volumes, depths and water retention times. Self-purification processes in lakes and reservoirs are controlled by the hydraulic behaviour of the water mass and by a series of other important factors, namely: dissolved oxygen supply, pH changes, water column stability and stratification residence time in the littoral region, particulate suspended and dissolved solids, including organic matter, temperature profiles, atmospheric loadings, nutrient and productivity controls depth and concentration gradients in aquatic eco-community. Thus, the physical processes of water quality hydrodynamics and transport mechanism associated with river are different than a lake or reservoir.

5.1.5 Challenges in surface water quality modeling

Water quality management is a critical component of overall integrated water resources management (Murty and Surender Kumar, 2011). Water quality can effectively be managed, if spatial and temporal variations of assimilative capacity of constituents and their transport mechanisms in a water body are known. Modeling as a management tool can give answer to assimilative capacity of constituents and waste load allocation as means of water-quality management along a water body wherein the amount of pollutant removal require at a number of discharge points can be determined. This can help achieve or maintain an acceptable level of water quality in an optimal manner. The other situation that may arise from the capacity expansion problem wherein one or more point sources has to increase in influent loading and the appropriate increase in the size of treatment facilities need to be determined. Another example may be the problem that occurs when an additional discharger wishes to locate on a water body that would necessitate a reallocation of the assimilative capacity of the water body among the existing dischargers (Burn, 1989) and so on.

Waste load allocation for water quality management can be accomplished by simulation and optimization modeling of hydrodynamic and transport behaviour of the water system through which contaminants move (McCutcheon, 1989). The prediction of water motion and the transport of materials impacting the water quality are carried out using some mathematical principles developed based on underlying mechanisms that cause change. The mathematical principles are to establish *cause-and-effect* relationships between sources of impurities, and the effects on water quality (Martin and McCutcheon, 1999). These relationships help us test hypotheses about a particular aquatic system, or process, aids in the diagnosis of factors contributing to particular water quality problems and help forecast the impacts of various environmental controls. The underlying *cause-and-effect* relationships are expressed mathematically by mechanistic models. In addition, empirical models such as; many statistical models allow description of the relationships with a minimum understanding about how the system works. However, the present-day models and modeling works encourage use of mechanistic models than empirical models; because empirical models are case specific and subjected to a lot of uncertainty although have a potential to associate with mechanistic models by their integration. Mechanistic models have three chief advantages (Martin and McCutcheon, 1999):

- Modeling allows researchers and scientists to gain insight and increased understanding of the water quality of a particular stream, lake and estuary;
- The process of calibrating mechanistic model not only provides information on cause-and-effect relationships, but also indicates what is not understood. Understanding the limits of knowledge about a particular water body is also important in making decisions about water resources,
- Most important is that mechanistic models provide a predictive capability that is not available in purely empirical models.

Water quality modeling deals with development and application of models by integrating the present understanding of transport and transformation of materials to predict the fate of those materials in the natural environment (Martin and McCutcheon, 1999). Water quality modellers construct and apply models that incorporate the present knowledge to test hypotheses, predict the effect of some action or solve a practical problem.

5.1.6 Status of surface water quality modeling in India

Ironically, surface water quality management issue in India is still to gear up for policy level planning, evaluation, and conservation measures. What has been emphasized in the past is water quality monitoring and quality assessment based on one-time monitored data of 2500 stations located in different rivers, lakes and groundwater wells. Water quality simulation modeling and management in India is a subject mostly dealt in academia and R & D organizations for specific research interest and knowledge gathering. Limited efforts are in place for strategic management of water quality problems. This could be due to the facts that; (i) there is inadequate spatio-temporal water quality data, which are not enough to conceive, calibrate and validate a model, (ii) lack of information/data on source of pollution and their magnitude and characteristics, (iii) lack of data on water quality hydrodynamics and kinetics, and (iv) lack of understanding of physical behaviour of the water system. Over the years, research investigations by different Indian researchers have generated considerable databases and knowledge understanding on water quality modeling of surface water systems. Further, Government of India has also launched "Ganga Rejuvenation" program with the vision to restore the wholesomeness of the river defined in terms of ensuring "Aviral Dhara" (Continuous Flow"), "Nirmal Dhara" ("Unpolluted Flow"), Geologic and ecological integrity. To achieve such goals, decisions are to be taken based on different water quality management scenario analyses. To a great extent, it is possible by pursuing/adopting suitable simulation-optimization models for water quality management as a scientific tool. The models should be such that they are appropriate for hydrodynamics and kinetics of Indian surface water systems, and can reasonably be used as decision support system for water quality management. This eventually advocates the need of evaluating the capability, performance, and effectiveness of existing widely used surface water quality models and strengthens the fitting model(s) by testing with Indian conditions.

5.2 Surface Water Quality Modeling: Importance

Increasing national and international interest in finding rational and economical approaches to water-quality management is one of the major issues in implementation of Water Framework Directive (WFD), particularly in terms of pollution control and management of water resources quality. Insightful application of mathematical models, attention to their underlying assumptions, and practical sampling and statistical tools can help maximize a successful approach to water-quality modeling. Mathematical modeling of water quality facilitates prediction of quantitative reaction and status of aquatic environments and impacts for defined pressures on aquatic environments, that is, human and natural activities in its surrounding. When correctly selected and used under strictly defined conditions and limitation, the mathematical model can play a very powerful tool in planning and management of water quality. Primarily, water quality models can serve for a quality interpretation of water resources status, and the causes of the status change can be detected. Further, the evaluation methods can be optimized. Secondly, these models can facilitate an analysis of the effects of future actions on the aquatic ecosystem and can support to the selection of the most sustainable options. Third, these models can assist in filling the gaps in our knowledge and defining a cost-effective monitoring program (Vanrolleghem *et al.*, 1999). Models help us gain insights into hydrological, ecological, biological, environmental, hydrogeochemical, and socioeconomic aspects of watersheds (Singh and Woolhiser, 2002), and thus contribute to systematized understanding of how ecosystems function (Lund and Palmer, 1997), which is essential to integrated water resources management and decision making (Madani and Marino, 2009).

Surface water pollution comprising rivers, lakes, reservoirs, ponds, etc is a major environmental problem in India that has negative consequences for humans and wildlife. To prevent its consequences, the sources and severity of pollution must be determined by monitoring water quality, followed by the measures necessary to control the contamination. Models are important tools for predicting adverse effects of pollution along a stream or in a water body, and they can help guide practical investments in stream health and management of surface water bodies.

While framing a mathematical model for surface water quality management, the purpose of modeling should be clear and well defined to achieve maximum simplicity consistent with the required degree of accuracy and detail in the process of description of the natural system. In general, the purpose of modeling falls into one of the following categories (Zheng and Bennett, 1995):

- In a scientific sense - to develop a clear conceptual model based on all available information as well as to understand more fully the transport regime of the pollutant:

to test hypotheses, to ensure that they are consistent with governing principals and observations, and to quantify the dominant controlling processes. Without this understanding, a simulation code can be used only as a black-box, and this clearly limits intelligent application of the model;

- Often in connection with efforts to assign responsibility or assess exposures, to reconstruct the history of pollutant transport, to establish time ranges within which an event could have begun, or within which contaminants could have reached specified level in certain areas;
- Future contaminant distributions, either under existing conditions or with engineering intervention to control the source or alter the flow regime, can be calculated. These include the choice of computer code, the way of discretization, the level of effort required in model calibration, and the analysis of the appropriated assumptions.

By definition of model, it is a simplified approximation to the real system. A simple model is always preferred than a complex model, as long as it captures the essence of the problem. An overly complex model not only increases computational time and costs, but also introduces additional uncertainties if detailed data are not available.

5.3 Modeling for Sustainable Water Quality Management

Water (and its deteriorating quality) is under the most severe stress due to the exponentially growing human population. Problems are becoming increasingly complex and diverse and require more and more specific knowledge and efficient integration across various disciplines, sectors, countries, and societies. The major challenge before us is to realize the desired integration and to resolve the large amount of existing gaps and barriers.

Challenges of water quality and quantity management adhering to the principle of sustainable development have been of significant concerns to many researchers and decision makers. These issues involve a large number of social, economic, environmental, technical, and political factors, coupled with complex spatial variability and cascading effect (Li et al., 2014). Climate change and human interference could affect the related management systems at a regional scale and lead to more significant spatial and temporal variations of water quantity and availability as well as the associated environmental and ecological conditions. Such complexities force researchers to develop more robust mathematical methods and tools to analyze the relevant information, simulate the related processes, implement mitigation strategies, assess the potential impacts/risks, and generate sound decision alternatives. Mathematical techniques can aid decision makers in formulating and adopting cost-effective and environment-benign water management plans and policies (Li et al., 2014).

In summary, the effective mathematical methods for modeling water quantity and quality are becoming one of the most important goals pursued by governments, industries, communities, and researchers. The contribution of degraded water to the water crisis, if measured in terms of loss of beneficial could be; water that is lost for beneficial human, agricultural, and ecological uses through excessive pollution by pathogens, nutrients, heavy metals and acid mine drainage, trace organic contaminants such as agricultural pesticides and pesticides associated with wood treatment, and localized high levels of oil and related pollutants, including salt, hydrocarbons, metals and other toxic wastes, and high levels of turbidity and sedimentation from excessive loadings of sediments. Therefore, to achieve the goal of sustainable water quality management, a number of issues involving identification, occurrence, and perception of various problems (e.g. eutrophication, acidification, global warming), pollution control types, wastewater treatment, modeling and monitoring, planning and environmental impact assessment, legislation and institutions, the notion of sustainable development, and the role of science and engineering, are to be addressed (UN-Water Analytical Brief).

5.4 Basic concept, Governing equations, Rate constants and Coefficients

5.4.1 Basic concepts

The fundamental principles for water quantity and quality modeling are (Chapra, 1997):

- Conservation of energy states (first law of thermodynamic);
- Conservation of mass states (mass balance models); and
- Conservation of momentum states (Newton's second law of motion).

These laws form the underlying principles of flow and water quality modeling. Conservation of energy is the basis of all mechanistic temperature modeling. Conservation of mass is the basis for transport modeling. When the mass balance is expanded to include kinetic changes of non-conservative parameters, these transport models are referred to as water quality models. Conservation of momentum is the basis for all flow models.

The basic principle underlying water quality modeling is that of mass balance. Modeling involves performing a mass balance for defined control volumes for a specified period of time. Typically, material balances involve dissolved and suspended materials such as dissolved oxygen, organic carbon, nitrogen, phosphorus, and suspended sediments and this principle is also applied to any substance whose transformation kinetics is known. The mass balance is performed by accounting for all material that enters and leaves a defined volume of water plus accounting for all changes in mass of a constituent caused by physical, chemical and biological processes. The conservation or balance equations in terms of mathematical statement can be stated as (Martin and McCutcheon, 1999):

$$\text{Accumulation} = \pm \text{Transport} \pm \text{Sources/Sinks} \qquad (5.1)$$

where accumulation is equal to the difference in transport into or out of a system, plus and gains or losses that resulted from sources and sinks. Accumulation is therefore the time rate of change by which a conservative property builds up or accumulates inside a system.

5.4.2 Governing equations

The mass conservation in a one-dimensional control volume where all processes act on it is depicted in Fig.5.1.

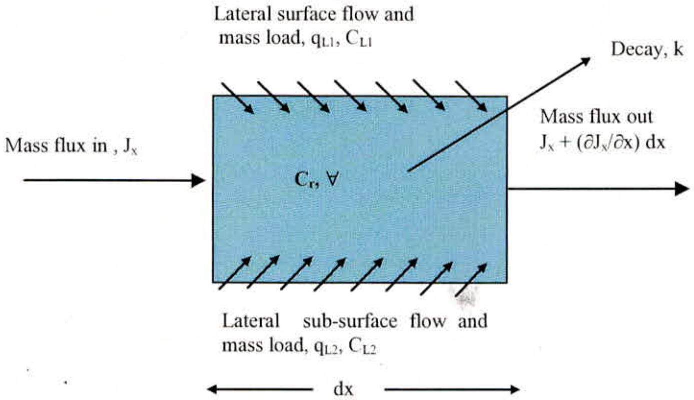

Figure 5.1: Mass conservation in a one-dimensional control volume.

Based on the basic principle of conservation of mass and the accumulation equation (eq. 5.1), the governing one-dimensional contaminant transport representing advective and dispersive mass fluxes, biochemical transformations, water column-sediment interactions, adsorption, external loadings, and change of mass of substance with time and space for a Newtonian fluid with constant density shown in Fig.5.1 is given by:

Rate of change of mass in control volume

Advective mass loading from surface lateral inflow

Advective mass loading from sub-surface lateral inflow

Dispersive mass loading from sub-surface lateral inflow

Mass influx

$$\frac{\partial (C_r \forall)}{\partial t} = q_{L1} C_{L1}\, dx + q_{L2} C_{L2}\, dx - n_{sed} D_{sed} \frac{C_{L2}-C_r}{\Delta z} w_r\, dx + \left(V\, A\, C_r - A\, D_x \frac{\partial C_r}{\partial x}\right) - \left[\left(V\, A\, C_r - A\, D_x \frac{\partial C_r}{\partial x}\right) + \frac{\partial}{\partial x}\left(V\, A\, C_r - A\, D_x \frac{\partial C_r}{\partial x}\right) dx\right] - k\, C_r \forall \tag{5.2}$$

Mass outflux

Biochemical decay

where, C_r is the mass density of a constituent (ML^{-3}); $\forall$ is the control volume (L^3);q_{L1} is the lateral surface discharge per unit length , ($L^3L^{-1}T^{-1}$); C_{L1} is the constituent concentration of lateral surface flow, (ML^{-3}); $q_{L2}$is the lateral subsurface discharge per unit length, ($L^3L^{-1}T^{-1}$); C_{L2} is the constituent concentration of lateral subsurface flow, (ML^{-3}); n_{sed} is the sediment porosity, (dimensionless); $w_r$is the width of the sediment layer at which the lateral subsurface flow takes place, (L); Δz is the thickness of the sediment layer, (L); D_{sed} is the dispersive properties of sediment, (L^2T^{-1}); V is the advective velocity of water along x direction, (LT^{-1}); A is the flow area, (L^2); D_x is the longitudinal dispersion coefficient, (L^2T^{-1}); k is the decay rate coefficient, (T^{-1}); dx is the length of the elementary stretch, (L); and$\partial C_r/\partial x$derivative of $C_r$with respect to x.

Simplification and rearrangement of Equation (5.2), gives:

$$\frac{\partial(C_r \forall)}{\partial t} = q_{L1} C_{L1}\, dx + q_{L2} C_{L2}\, dx - n_{sed}\, D_{sed}\, \frac{C_{L2}-C_r}{\Delta z} w_r\, dx - \frac{\partial}{\partial x}\left(V\, A\, C_r\, - A\, D_x \frac{\partial C_r}{\partial x}\right) dx - k\, C_r A\, dx \qquad (5.3)$$

In terms of mass transport, considering $M = C_r\ \forall$, Equation (5.2) can be written as:

$$\frac{\partial M}{\partial t} + \frac{\partial}{\partial x}(VAC_r)\, dx\ = \frac{\partial}{\partial x}\left(A\, D_x \frac{\partial C_r}{\partial x}\right)\, dx - \ k\, C_r A\, dx\ +\ q_{L1} C_{L1}\, dx + q_{L2} C_{L2}\, dx\ - n_{sed}\, D_{sed}\, \frac{C_{L2}-C_r}{\Delta z} w_r\, dx \qquad (5.4)$$

When there is no contribution from lateral inflows, Equation. (5.4) represents well known contaminant transport equation in one-dimension that is used for river contaminant transport modeling:

$$\frac{\partial M}{\partial t} + \frac{\partial}{\partial x}(VAC_r)\, dx\ = \frac{\partial}{\partial x}\left(A\, D_x \frac{\partial C_r}{\partial x}\right) dx\ -\ k\, C_r A\, dx \qquad (5.5)$$

The three dimensional governing equation representing advective and dispersive mass fluxes, biochemical transformations, sources and sinks, and change of mass of the substance with time and space, based on Equation. (5.5) is given by:

$$\frac{\partial M}{\partial t} + \frac{\partial(V_x A_x C_r)}{\partial x}\, dx + \frac{\partial(V_y A_y C_r)}{\partial y} dy + \frac{\partial(V_z A_z C_r)}{\partial z} dz = \frac{\partial}{\partial x}\left(A_x\, D_x \frac{\partial C_r}{\partial x}\right)\ dx + \frac{\partial}{\partial y}\left(A_y\, D_y \frac{\partial C_r}{\partial y}\right) dy + \frac{\partial}{\partial z}\left(A_z\, D_z \frac{\partial C_r}{\partial z}\right)\ dz \pm\ k(x,y,z,t)\, C_r\, dx\, dy\, dz \pm S \qquad (5.6)$$

In which, M is the mass of constituents, (M); D_x, D_y, and D_z are the dispersive mass fluxes in the spatial directions x, y, and z ($L^{-2}\ T^{-1}$);V_x, V_y, and V_z are the components of the flow velocity in spatial directions x, y, and z ($L\ T^{-1}$); A_x, A_y, and A_z are the cross-sectional area of the control volume in directions x, y, and z, (L^{-2});t is time (T); *dx, dy,* and *dz* are the dimension of the control volume in direction x, y, and z, (L); ∂x, ∂y, and ∂z are the derivative in direction x, y, and z;*k(x,y,z,t)* is the growth and decay coefficients of the constituent, (T^{-1}); andS is the external sources and sinks of the constituent, ($M\ L^{-3}\ T^{-1}$).

Organic matters undergo changes because of air-water interface and nutrients interactions into the water body. The air-water interface and nutrients interactions affect the water temperature, dissolved oxygen, Nitrogen, and Phosphorous cycle, which in turn, change the fate of water quality constituents and also the ecology of water system. Fig. 5.2 depicts the interactions of constituents of organic matters in a surface water body. For management of water quality and ecology of a surface water system, one has to know the fate of the organic constituents' concentration on spatial and temporal scale.

Lake water quality modeling deals with two components: hydrodynamic and pollutant transport. The governing system of equations for the flow and transport in a lake include the conservation equations of mass, momentum and energy. The contaminant transport equation is based on the conservation of mass and Equation. 5.6 holds good for lake water quality modeling. For hydrodynamic modeling, conservation of momentum, mass and energy provide the fundamental principles.

The major difference between rivers and lakes is in the speed of water flow. Water speeds are generally much smaller in lakes than in rivers. Thus, in Equation 5.6, the advection term is generally much larger than the mixing term in rivers, while the advection term may be comparable to or even smaller than the mixing term in lakes. Lakes are also distinguished from estuaries that have interchanges with the ocean and are subject to tide.

Due to its relatively large velocity, a river, especially a shallow and narrow river, can often be represented by one-dimension. By contrast, a lake generally has much more complicated circulation patterns and mixing processes, which are largely affected by lake geometry, vertical stratification, hydrological and meteorological conditions. Lakes and reservoirs tend to store water over seasons and years. Such a long retention time often makes internal chemical and biological processes significant in the lake water column and the sediment bed. Thus, the hydrodynamic modeling of a lake is much complicated than the transport modeling, however, without hydrodynamic modeling, a transport modeling cannot be addressed.A variety of factors control the in-lake hydrodynamic condition, they include: (i) depth, length, width, volume, and surface area; (ii) inflows and outflows; (iii) hydraulic residence time; and (iv) lake stratification.

Lakes and reservoirs are sensible to pollutants from point and non-point sources. Lake eutrophication by the excessive algal growth and low DO levels are common symptoms originate from excessive nutrient loadings, namely Nitrogen and Phosphorous.The interactions of organic constituents depicted in Fig. 5.2 also hold good for Lake eutrophication modeling.

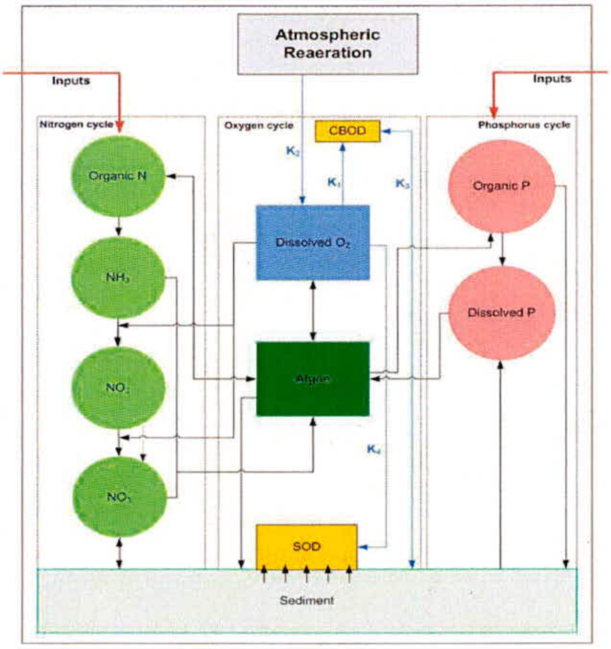

Figure 5.2: Interactions of organic constituents in a water body.

The chemical and biological processes and their reaction kinetics are temperature dependant. These processes can be modeled by first-order kinetic equations.

5.4.3 Temperature

Temperature impacts almost all water quality processes that take place in a water body. Temperature is modelled by performing a heat balance on each computational element in the system. The simplified model for temperature prediction is:

$$\frac{dT}{dt} = \frac{K_H(Te-T)}{\rho C_P h} \qquad (5.7)$$

where K_H (cal/cm^2/day/°C) is the overall heat exchange coefficient; *Te* (°C) is the equilibrium temperature; T (°C) is actual temperature; ρ (g/cm^3) is the water density; *Cp* (cal/g/°C) is the heat capacity of water; and *h* (cm) is the water depth.

The temperature computed by Equation 5.7 is used to correct the rate coefficients of the source/sink terms of the water quality variables. Generally, these coefficients are determined at controlled temperature of 20ºC. The correction to the rate coefficient for temperature is:

$$X_T = X_{20}\,\theta^{T-20°} \qquad (5.8)$$

Where X_T is the value of the coefficient at the desired temperature [T]; X_{20} is the value of the coefficient at the standard temperature (20ºC); and θ is an empirical constant for each reaction coefficient.

5.4.4 De-oxygenation model

De-oxygenation is the process that involves the removal of oxygen from water. In water quality modeling, it describes how dissolved oxygen (DO) in water decreases by degradation of biochemical oxygen demand (BOD). Mathematically, the deoxygenating equation is described by first order kinetics, as follows:

$$\frac{dL}{dt} = -K_1 L \qquad (5.9)$$

in which, L is the BOD concentration, [ML^{-3}]; K_1 is the de-oxygenation rate coefficient and is temperature dependent, [T^{-1}].

5.4.5 Re-aeration model

Re-aeration is the process of oxygen exchange between the atmosphere and water body in contact with the atmosphere. The re-aeration process is modelled as the product of a mass transfer coefficient multiplied by the difference between dissolved oxygen saturation and the actual dissolved oxygen concentration, that is:

$$\frac{dC}{dt} = K_2(C_s - C) \qquad (5.10)$$

where C is the concentration of oxygen in water volume, [ML^{-3}]; C_S is the saturated concentration of oxygen in water volume, [ML^{-3}]; K_2 is the re-aeration coefficient, and is temperature dependent, [T^{-1}].

5.4.6 BOD and DO model

Streeter and Phelps (1925) established the relationship between the decay of organic waste measured in terms of BOD and dissolved oxygen (DO). The relation between the DO and BOD concentration over time is modelled by the linear first order differential equation, as follows:

$$\frac{dD}{dt} = -K_1 L - K_2 D \qquad (5.11)$$

where D is the dissolved oxygen (DO) deficit, $[ML^{-3}]$; K_1 and K_2 represent the de-oxygenation and re-aeration rate coefficient, respectively and they are temperature dependent $[T^{-1}]$

The solution of Equation 5.11 gives the well known DO sag model:

$$D = \frac{K_1 L_0}{K_2 - K_1}(e^{-K_1 t} - e^{-K_2 t}) + D_0 e^{-K_2 t} \qquad (5.12)$$

where, $L_0$is the initial oxygen demand of organic matter in the water, also called the ultimate BOD, $[ML^{-3}]$; D_0 is the initial DO deficit, $[ML^{-3}]$; and $D = DO_{sat} - DO$.

The DO processes which involve consumption and release of oxygen in receiving water are described by Equation 5.13 (Palmer, 2001). Equation 5.13 expresses DO as sum of the sources i.e, re-aeration & algal production and sinks i.e, BOD, sediment oxygen demand (SOD) and nitrogen oxidation.

$$\frac{dDO}{dt} = K_2 (DO_{sat} - DO) + (\alpha_3 \mu - \alpha_4 \rho)A - K_1 L - \frac{K_4}{H} - \alpha_5 \beta_1 N_1 - \alpha_6 \beta_2 N_2 \qquad (5.13)$$

where, K_2 is the re-aeration rate coefficient $[T^{-1}]$; α_3 is the rate of oxygen production per unit of algal photosynthesis;α_4 is the rate of oxygen uptake per unit of algal respired; α_5 is the rate of oxygen uptake per unit of ammonia nitrogen;$\alpha_6$is the rate of oxygen uptake per unit of nitrite nitrogen; μ is the growth rate of algae, $[T^{-1}]$; ρ is the algal respiration rate, T^{-1}; A is the algal biomass concentration, $[ML^{-3}]$; H is depth(m);K_4 is sediment oxygen demand $[ML^{-2}T^{1}]$; β_1 is the rate constant for biological oxidation of ammonia nitrogen, temperature dependent, $[T^{-1}]$; N_1 is the concentration of ammonia nitrogen, $[ML^{-3}]$; β_2 is the rate constant for oxidation of nitrite nitrogen, temperature dependent, $[T^{-1}]$; N_2 is the concentration of nitrite nitrogen, $[ML^{-3}]$.

5.4.7 Nutrients model

In water quality modeling, nitrogenous and phosphorous compounds play important roles as they consume oxygen during oxidation processes in conversion of different forms i.e., nitrogen and phosphorous cycle (USEPA, 1987). Fig. 5.2 describes the constituents' interactions in the nitrogen and phosphorous cycle.

5.4.8 Nitrogen cycle

In natural aerobic waters, there is a stepwise transformation from organic nitrogen to ammonia, to nitrite, and finally to nitrate. The differential equations governing transformations of nitrogen from one form to another are given by (USEPA, 1987).

5.4.8.1 Organic Nitrogen Model

Referring to Fig. 5.2, the organic Nitrogen model is described as:

$$\frac{dN_4}{dt} = \alpha_1 \rho A - \beta_3 N_4 - \sigma_4 N_4 \qquad (5.14)$$

where N_4 is the concentration of organic nitrogen, [M-N L^{-3}] ; β_3 is the rate constant for hydrolysis of organic nitrogen to ammonia nitrogen, temperature dependent, [T^{-1}]; α_1 is the fraction of algal biomass that is nitrogen, (M-N/M-A); ρ is the algal respiration rate, day^{-1}; A is the algal biomass concentration, (M-AL^{-3}); and σ_4 is therate coefficient for organic nitrogen settling, temperature dependent, [T^{-1}].

5.4.8.2 Ammonia Nitrogen Model

Referring to Fig.5.2, the Ammonia Nitrogen model is described as:

$$\frac{dN_1}{dt} = \beta_3 N_4 - \beta_1 N_1 + \frac{\sigma_3}{d} - F_1 \alpha_1 \mu A \qquad (5.15)$$

where $F_1 = \frac{P_N N_1}{(P_N N_1 + (1 - P_N) N_3)}$; N_1 is the concentration of ammonia nitrogen, (M-NL^{-3});N_3 is the concentration of nitrate nitrogen, (M-NL^{-3}); N_4 is the concentration of organic nitrogen, (M-NL^{-3}); β_1 is the rate constant for biological oxidation of ammonia nitrogen, temperature dependent, [T^{-1}]; β_3 is the organic nitrogen hydrolysis rate, [T^{-1}]; α_1 is the fraction of algal biomass that is nitrogen, (M-N/M-A); σ_3 is the benthos source rate for ammonia nitrogen, M-N/L^2-day; d = mean depth of flow, [L]; μ is the local specific growth rate of algae, [T^{-1}]; F_1 is the fraction of algal biomass that is nitrogen, mg-N/mg-A; A is the algal biomass concentration, M-A/L^3; and P_N is the preference factor for ammonia nitrogen (0 to 1.0). The ammonia preference factor is equivalent to the fraction of algal nitrogen uptake from the ammonia pool when the concentration of ammonia and nitrate nitrogen is equal.

5.4.8.3Nitrite Nitrogen Model

Referring to Figure 2, the Nitrite Nitrogen model is described as:

$$\frac{dN_2}{dt} = \beta_1 N_1 - \beta_2 N_2 \qquad (5.16)$$

where N_1 is the concentration of ammonia nitrogen, M-N/L^3; N_2 is the concentration of nitrite nitrogen, M-N/L^3; β_1 is therate constant for oxidation of ammonia nitrogen, temperature dependent, (T^{-1}); β_2 is the rate constant for oxidation of nitrite nitrogen, temperature dependent, (T^{-1}).

5.4.8.4 Nitrate Nitrogen Model

Referring to Fig.5.2, the Nitrate Nitrogen model is described as:

$$\frac{dN_3}{dt} = \beta_2 N_2 - (1 - F) \alpha_1 \mu A \qquad (5.17)$$

where F is the fraction of algal biomass that is nitrogen, M-N/M-A; α_1 is the fraction of algal biomass that is nitrogen, M-N/M-A; and μ is the local specific growth rate of algae, (T^{-1}).

5.4.8.5 Phosphorous Cycle

Organic forms of phosphorous are generated by the death of algae, which then convert to the dissolved inorganic state, where it is available to algae for primary production. Fig. 5.2 refers the constituents' interactions in the Phosphorous cycle.

5.4.8.6 Organic Phosphorous Model

The differential equation representing the organic Phosphorous model is given by:

$$\frac{dP_1}{dt} = \alpha_2\rho A - \beta_4 P_1 - \sigma_5 P_1 \quad (5.18)$$

where P_1 is the concentration of organic phosphorous, M-P/L; $\alpha_2$is the phosphorous content of algae, M-P/M-A; ρ is the algal respiration rate, $[T^{-1}]$; A is the algal biomass concentration, M-A/L; β_4 is the organic phosphorous decay rate, temperature dependent, $[T^{-1}]$; σ_5 is the organic phosphorous settling rate, temperature dependent, $[T^{-1}]$.

5.4.8.7 Dissolved Phosphorous

The differential equation for modeling dissolved Phosphorous is given by:

$$\frac{dP_2}{dt} = \beta_4 P_1 - \sigma_2/d - \alpha_2\mu A \quad (5.19)$$

where $P_2$is the concentration of inorganic or dissolved phosphorous, M-P/L; σ_2 is the benthos source rate for dissolved phosphorous, temperature dependent, M-P/L-T; d is the mean stream depth, [L]; $\mu$is the algal growth rate, $[T^{-1}]$; and A is the algal biomass concentration, M-A/L.

5.4.9 Coliform

Coliforms are used as an indicator of pathogen contamination in surface waters. Expressions for estimating coliform concentrations are usually first order decay functions, which only take into account coliform die-off (Bowie et al., 1985) and can be expressed as:

$$\frac{dE}{dt} = K_5 E \quad (5.20)$$

where E is the concentration of coliforms, colonies/100 ml; and K_5 is the coliform die-off rate, temperature dependent, (T^{-1}).

5.4.10 Algae formulation

Chlorophyll_a is considered to be directly proportional to the concentration of phytoplanktonic algal biomass. In modeling, algal biomass is converted to Chlorophyll a by the simple relationship:

$$Chl\_a = \propto_0 A \quad (5.21)$$

where Chl_a is the Chlorophyll_a concentration , M-Chl_a/L; A is the algal biomass concentration, M-A/L;$\propto_0$ is a conversion factor (M-Chl_a/M- A).

The differential equation that governs the growth and production of algae (Chlorophyll_a) is formulated according to the following relationship:

$$\frac{dA}{dt} = \mu A - \rho A - \frac{\sigma_1}{d} A \quad (5.22)$$

where t is the time, [T]; μ is the local specific growth rate of algae, which is temperature dependent, $[T^{-1}]$; ρ is the local algal respiration rate, which is temperature dependent, $[T^{-1}]$; σ_1 is the local settling rate for algae, which is temperature dependent, $[LT^{-1}]$; and d is the mean stream depth, [L].

5.5 Approaches to Surface Water Quality Modeling

5.5.1 Rivers/Stream water quality modeling

Except the initial mixing length from the entry of point source pollution, contaminant transport in a river/stream is normally one-dimensional. In the initial period of mixing, contaminant transport is governed by 3-dimension. River/stream contaminant transport equation in one-dimension governed by advection-dispersion-decay/growth-sorption and sources/sinks can be modelled by Equation 5.6 neglecting y and z directional components, i.e., by considering $V_y = V_z = 0; D_y = D_z = 0$, and $y = z = 0$.

For one-dimensional transport modeling, the data requirements are: (i) river/stream geometry (width, depth and slope); (ii) river/stream hydraulic data (cross-sectional average velocity, and flow rate); (iii) transport properties (longitudinal dispersion coefficient, reaction kinetics, water temperature, and initial concentration of contaminants of interest; sources and sinks of contaminant in the system); (iv) ambient temperature; (v) concentration of organic constituents; and (vi) input stresses of contaminant.

These data are case specific and vary from one river to another and can be obtained from field and laboratory investigations. The estimation of longitudinal dispersion coefficient, D_x or D_L, that depends on river/stream hydraulic properties and mixing phenomena of contaminant, and may vary from location to location, is not a straight forward approach. Methods suggested by different investigators for estimation of D_L are listed in Table 5.1.

Table 5.1 Methods suggested by investigators for estimation of D_x (Source: Ghosh, 2000; and Muthu Krishnavellaisamy, 2007)

Sl. No.	Investigators	Equation	Method
1.	Taylor (1921)	$\frac{d\sigma^2}{dt} = 2D$; where, σ^2 is the variance of solute distribution and D is the diffusion co-efficient.	Experimental
2.	Chatwin (1971), and Valentine and Wood (1979)	$D_L = \frac{\bar{u}^3}{2}\frac{d\sigma_t^2}{dx}$ where, $\bar{u}$ is the average flow velocity, σ_x is the spatial variances of concentration distribution.	Experimental
3.	Elder (1959)	$D_L = \left[\frac{0.404}{\kappa^3} + \frac{\kappa}{6}\right] yU_*$ where κ is the Von Karman's coefficient, and U_* is the shear velocity, and y is the vertical distance.	Theoretical
4.	Fischer *et al.*, (1979)	$D_L = -\frac{1}{A}\int_0^B u' y \int_0^y \frac{1}{\varepsilon_t y} \int_0^B u' y dy dy dy$ where u' is the deviation of velocity from the cross sectional mean velocity, y is the depth of flow, and ε_t is the transverse mixing coefficient.	Theoretical
5.	Taylor (1954)	$D_L = 10.1\ U_* r$ where$U_*$is the shear flow velocity , and$r$ is the radius of the pipe.	Empirical
6.	Elder (1959)	$D_L = 6.3\ U_* H$ where H is the depth of flow	Empirical
7.	Yotsukura and Fiering (1964)	$D_L = 9.0 \text{ to } 13.0\ U_* H$	Empirical
8.	Fischer (1966)	$D_L = 0.011\ u^2\ W^2 / U_* H$ where W is the width of he stream, and u is the mean flow velocity.	Empirical
9.	Thackston and Krenkal (1967)	$D_L = 7.25\ U_* H \{u / U_*\}^{1/4}$	Empirical
10.	Sumer (1969)	$D_L = 6.23\ U_* H$	Empirical
11	Fukuoka and Sayre	$D_l / RU_* = 0.8\{r_c^2 / L_B H\}^{1.4}$	Empirical

Sl. No.	Investigators	Equation	Method
	(1973)	where R is the hydraulic depth, r_c is the	
12.	McQuivey and Keefer(1974)	$D_L = 0.058\ Q/SW$	Empirical
11.	Jain (1976)	$D_L = u^2\ W^2 /k\ AU_*$	Empirical
12.	Beltaos (1978)	$D_L/RU_* = \alpha\ \{W/R\}^2$	Empirical
13.	Liu (1977)	$D_L = Q^2/2U_*R^3\ \{U_*/u\}^2$	
14.	Magazine (1983)	$D_L/R_bU_* = D_L/R_wU_* = 75.86\ (Pr)^{1.632}$ Where $Pr = C_w/\sqrt{g}\ \{x/h\}^{0.3}\{x_1'/b\}^{0.3}\{1.5+e/h\}$	Empirical
15.	Marivoet and Craenenbroec (1986)	$D_L = 0.0021\ u^2\ W^2/U_*H$	Empirical
16.	Asai *et al.* (1991)	$D_L/\ U_*H = 2.0\ \{W/R\}^{1.5}$	Empirical
17.	Ranga Raju *et al.* (1997)	$D_L/qS = 0.4\ Pt$ Where $Pt = \{W/R\}^{2.16}\{u\ /\ U_*\}^{-0.82}\{S\}^{-0.2}$	Empirical
18.	Koussis and Mirasol (1998)	$D_L = \Phi \sqrt{}\ (gRS)/H\ \{W\}^2$	Empirical
19.	Seo and Cheong (1998)	$D_L/U_*H = 5.915\{W/H\}^{0.628}\{u/\ U_*\}^{1.428}$	Empirical
20.	Kezhong and Yu (2000)	$D_L/U_*H = 3.5\{W/H\}^{1.125}\{u/\ U_*\}^{0.25}$	Empirical

Empirical formulae indicate that D_L is a function of stream flow characteristic and stream geometry. By analyzing empirical formulae, Seo and Cheong (1998) suggested a generalized functional relationship of D_L with flow characteristic and geometry of a stream of the following form:

$$\frac{D_L}{U_* H} = a\left(\frac{W}{H}\right)^b \left(\frac{u}{U_*}\right)^c \tag{5.23}$$

where W is the river width, H is the depth of the flow, u is the mean longitudinal velocity, U_* is the shear velocity, $(=\sqrt{\mathrm{gRS}}$;where g is the gravitational acceleration constant; R hydraulic radius (flow area/wetted perimeter); and S is the friction slope ($S \approx \partial h/\partial x \approx$ bed slope) (Bashitialshaaer *et al.*, 2011), and *a, b, c* are constants.

The parameters of reactive kinetics viz., decay rate coefficient, sorption kinetic coefficients, benthic kinetic coefficient; kinetic coefficients related to Nitrogen and Phosphorous cycle, algal and coliform cycle can be determined from the field and laboratory experiments.

5.5.2 Lake and estuary water quality modeling

Lake and estuary water quality modeling is a complicated and tedious job. It involves numerical approach towards hydrodynamic and pollutant transport modeling in 3-dimension. Hydrodynamic and pollutant transport processes are mathematically modelled using field observations and laboratory experimental data, as illustrated in Fig.5.3.

5.6 A Review of different modeling approaches

Surface water quality models have undergone a long period of development since Streeter and Phelps built the first water quality model (S-P model) to control river pollution in Ohio State of the US (Streeter and Phelps, 1925). More than 100 surface water quality models have been developed up to now (Wang *et al.*, 2013). The models developed, to deal with real life issues, field complexity, research interest, and water quality management, forriver/stream water quality modeling include: Empirical or Mechanistic models, Conceptual models, Processes based models, Stochastic models, Analytical models, Numerical models, Black-box models and Stream tube models.

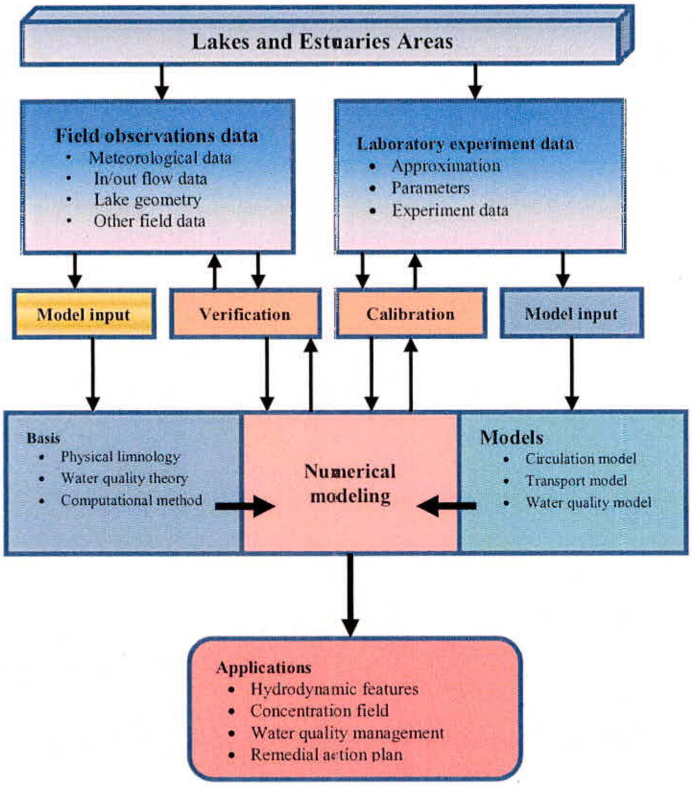

Figure 5.3: Schematic diagram of approaches for lake/estuary numerical hydrodynamic and transport modeling (source: modified from Tsanis and Wu, 1994)

5.6.1 Empirical and mechanistic models

The models are often divided into two broad categories as empirical and mechanistic depending on the way in which they influence the determinants, but the distinction is not clear-cut and mechanistic descriptions will often contain empirically derived components (Cox, 2003). The empirical models make no attempt to explicitly model hydrochemical processes; instead the model inputs are related directly to its outputs by one or more relationships obtained experimentally. Empirical models are derived by curve fitting or statistical analysis of stream/river data defining a process of interest, while a mechanistic model is formulated on a hypothesis of controlling mechanism. By contract, a mechanistic model is different from empirical model by statistical analysis without regard to controlling mechanisms. In mechanistic models, the transfer of water and solutes between stores is governed by mass-balance budgeting. As a result, mechanistic models are evidently equivalent to theoretical and phenomenological models.Any good model has both empirical and mechanistic features.

Examples: (i) Empirical models for estimating the concentration and exports of metals in rural rivers and streams developed by Cuthbert and Kalff (1993); (ii) Empirical regression models for prediction of nutrient export specific to the Muskoka-Haliburton area of Central Ontario; (iii) Streeter and Phelps oxygen sag model (1925) is a mechanistic model; (iv) Biofilm consumption model is a mechanistic model (Lau, 1990).

5.6.2 Conceptual models

A conceptual model describes essential features of a phenomenon and identifies the principal processes taking place in it. Thus, the conceptual models represent physical processes and also statistical and empirical relationships to process-based and physically-based models derived from physical and physicochemical laws including some equations based on empirical knowledge. Simplified conceptual models sometime suffer from a lack of description of physical processes.

Example: Almost all numerical river water quality models are conceptual models, viz. QUAL series, WASP series, SWAT, MIKE series models, etc. Cells-in-series (Stefan and Demetracopoulos, 1981), Hybrid-cells-in-series (Ghosh *et al.*, 2004), Aggregated Dead Zone (ADZ) model (Beer and Young, 1984), etc are conceptual models for solute transport in one-dimensional stream/river.

5.6.3 Process based models

Process-based models (sometimes known as deterministic or comprehensive models) are those, which are derived based on the mathematical representation of one or several processes characterizing the functioning of the natural system using mainly on mathematical representation of physical laws on the flow of mass, momentum and energy. As a rule, a physically based model has to be fully distributed, and has to account for spatial variation of all variables.

Examples: SWAT and SWIN model,

5.6.4 Stochastic models

Stochastic models incorporate the inherent uncertainty of models by describing the central tendency and some measures of variability of parameters. This results in a probability density function for the prediction. Stochastic models sometimes use empirical description of parameter variability. Monte Carlo simulation, Markov chain, Kalman filter, Fokker-Planck equation, etc are used for stochastic water quality modeling.

Examples: SORM-Stochastic River Water Quality Model.

5.6.5 Analytical models

Analytical models are those that are based on analytical solution of the governing equations. Analytical models are based on exact solutions of the equations of mathematical physics. The plug-flow solution of the dissolved oxygen balance equation, known as the Streeter –Phelps equation, is perhaps the best known analytical model in stream modeling. In analytical modeling, the model parameters in a reach remain constant. The Ogata and Banks solution for the one-dimensional advection-dispersion equation is well known analytical model for solute transport in stream modeling. Analytical solutions are quite limited use and are very useful to verify numerical solution techniques.

Examples: Streeter and Phelps model, Ogata and Banks solution (1963) of 1-D ADE, etc.

5.6.6 Numerical models

The numerical models are those that require finite difference, finite element, and other approximate methods for solving water quality equations. Numerical models use approximate solutions. They are used in most general purpose stream water quality models. Almost all commercial and public domain water quality models are based on numerical solutions.

Examples: QUAL2E, WASP, MIKE, etc.

5.6.7 Black-box models

Lumped models are also referred as the Back-box models. Lumped-parameter models refer to the absence of space-dependency, therefore, they are zero-dimensional in space; they are based on an assumption of uniform conditions throughout the system modelled.

5.6.8 Stream tube models

The fundamental concept of stream tube model was given by Yotsukura and Cobb in the year 1972 considering the cumulative partial discharge at a given cross-section instead of lateral distance as independent variable by dividing the cross-section into a number of vertical strips termed as "stream tubes". In the traditional approach, the strips are equal to width. Later on, Gowda (1980) extended it for water quality prediction in mixing zones of shallow rivers. In the stream tube model, analytical solutions of the steady state, 2-D convection-diffusion equation are modified to account for the longitudinal variability of decay and dispersion parameters. Stream tube models have not gained popularity like other modeling approaches.

5.7 An Appraisal of WaterQuality Models

The water quality models have come a long way and a wide variety of models are available today for assessment and management of water quality of rivers, reservoirs, lakes, estuaries, and watersheds worldwide. The assessment of water quality, understanding of its transport mechanism, simulation & prediction of transport processes and optimization of engineering interventions to control pollution, involve good databases for developing and/or selecting a suitable model. Mathematical modeling has become the standard procedure especially in characterizing and investigating water quality management problems in water bodies (Bath *et al.*, 1997; Chapra, 1997; Fitzpatrick *et al.*, 2001; Imhoff, 2003). Cox (2003) states that a great deal of work and time would be saved if an existing model suitable for the purposes of the study is chosen based on the data requirements and the appropriateness to deal with the water quality management problem at hand. Tsakiris and Alexakis (2012) suggested criteria for classification of water quality models as: (i) type of approach: physically based, conceptual, and empirical; (ii) pollutant item: nutrients, sediments, salts etc.; (iii) area of application: catchment, groundwater, river system, coastal waters, integrated; (iv) nature: Deterministic or Stochastic; (v) state analysed :steady state or dynamic simulation; (vi) spatial analysis: lumped, distributed; (vii) dimensions: 1-D or 2-D models; and (viii) data requirements: extensive databases, minimum requirements models (MIR).

Based on the approaches of modeling, numerous professional water quality models developed in the past have been complied and discussed in length by a number of researchers (Palmer, 2001; Riecken, 1995; Wang, 2013; Zieminska-Stolarska, 2012). Table 1 provides a list of some professional "*Water Quality Models*" with their special characteristics. These models are listed in three categories: (i) models applicable to assist transport of contaminants exclusively for catchment/watershed, (ii) models applicable for simulation of contaminants' transport in rivers/streams, and (iii) models applicable for contaminants transport modeling in rivers, lakes, estuaries and wetlands. A critical appraisal of each of these models based on the environment modelled, basic principle and process description, assumptions, data inputs and requirements, modeling capability, level of complexity, scale of their use, availability, degree of uncertainty, and their strengths and weaknesses, is presented here to help identify the "*most suitable water quality models*" for developing countries like India for sustaining the ever deteriorating water quality in the arena of urbanisation, industrialization, climate change, and to secure "Clean and Continuous Water Supplies" for ever-growing population.

According to Whitehead (1980), while critically appraising the water quality models, stated that an ideal model should qualify the following criteria:

(a) It should be a truly dynamic model capable of accepting time-varying inputs of the upstream water quality, which are used to compute time varying output responses downstream;
(b) It should provide a reasonable mathematical approximation of the physical, chemical and biological changes occurring in the river system and should be compared with real data collected from the river at a sufficiently high frequency and for a sufficiently long period of time;
(c) The model should be as simple as possible whilst retaining the ability to adequately characterize the important aspects of the system behaviour;
(d) It should be able to account for the inevitable errors associated with laboratory analysis and sampling, and account for the uncertainty associated with imprecise knowledge of the pertinent physical, chemical and biological mechanisms.

Table 5.2 summarizes a total of 27 water quality models, out of which 16 have been grouped into rivers, lakes, reservoirs, watershed and estuaries, wetlands category and 11 models specifically for river water quality modeling. If we critically examine Table 1 on the basis of modeling capability, processes involved and data requirement, then AQUATOX, DYRESM 1D, and MINLAKE models can be specifically used for lakes and reservoirs, and TSM, for lakes only. The AQUATOX is the simplest model and is available in free domain, and can simulate nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants, while DYRESEM 1D and MINLAKE are license based and hydro-dynamic in nature and could be classified as complex and intermediate complex models. Based on modeling capabilities, the AQUATOX can be preferred over MINLAKE and DYRESEM 1D models.

The models, such as BASINS, ECM, EUTROMOD and HSPF, are used for water quality modeling of watersheds, lakes and streams. In these models, the BASINS and HSPF models can be specifically used for NPS water quality modeling of watersheds and in-streams and lakes, respectively. The HSPF model is very data intensive, and can be explored for detailed water quality analysis of watersheds, lakes and streams.

The model simulates detailed watershed temperatures and concentrations of various water quality constituents in river (Gao and Li, 2014).The ECM and EUTROMOD models, though have comparatively lower data requirements, but have very limited applicability. The ECM model has been used in predicting the total amount of phosphorus and nitrogen (Bowes *et al.* 2008, European Commission 2003 a-c). The EUTROMOD model has limited applications in lake water quality modeling.

The models such as, CE-QUAL-W2, EFDC, COASTOX, and WASP7 can simulate simultaneously the water quality of rivers, lakes, reservoirs, wetlands, estuaries, and coastal ocean regions. The models like CE-QUAL-W2, EFDC and WASP has been widely used in water quality modeling worldwide (Gao and Li, 2014). WASP is one of the most widely used water quality models in the United States and throughout the world. Because of the models capabilities of handling multiple pollutant types, it has been widely applied in the development of Total Maximum Daily Loads (TMDL). However, the use of COASTOX model has been found limited in water quality modeling. MIKE 11 has been wildly used by researchers mainly for rivers and lakes. It operates on a number of timescales from single storm events to monthly water balance. A common problem with complex process models like MIKE 11 is the need of large amounts of data that may not be available in many situations, like in Indian conditions.

The WASP model can be combined with EUTRO and TOXI to simulate eutrophication, nutrient, metals, toxics, and sediment transport. The model has a user-friendly windows-based interface with a pre-processor; sub-model processors and a graphical postprocessor. WASP has capabilities of linking with hydrodynamic and watershed models, which allow for multi-year analysis under varying meteorological and environmental conditions. The outputs of WASP can be transferred to programs used for Geographical Information System (GIS) and water quality statistics. MIKE 11 model is an advanced model of flow and water-quality in stream and can simulate solute transport and transformation in complex river systems. Although a promising model, but its large data requirement, complex computational processes, long computational times and licensing put a limiting condition to MIKE11 for large scale uptakes

Table 5.2 A list of some Surface Water Quality Models with their special characteristics

Sl. No.	Model	Dimensions and State of Hydraulics	Pollutant type it can handle	Description	Year of Development & by whom	Open /license	Applicability	Reference
RIVERS, LAKES, RESERVOIRS, WATERSHED AND ESTUARIES WATER QUALITY SIMULATION MODELS								
1	**AQUATOX**	2-Dimensional, dynamic model	It predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants.	AQUATOX is a PC based ecosystem model that predicts the fate of nutrients, sediments, and organic chemicals in water bodies, as well as their direct and indirect effects on the resident organisms.	Developed in year 2003 and latest release 3.1 was in year 2014 by the US-EPA	Open	Lakes and reservoirs.	Center for Exposure Assessment Models (CEAM), US-EPA.
2	**CE-QUAL-W2**	2-Dimensional(longitudinal-vertical)hydrodynamic	It can simulate eutrophication processes such as temperature-nutrient-algae-dissolved oxygen-organic matter and sediment relationships.	It considers longitudinal-vertical hydrodynamics and water quality in stratified and non-stratified systems, nutrients-dissolved oxygen-organic matter interactions, fish habitat, selective withdrawal from stratified reservoir outlets, hypolimneticaeration, multiple algae, epiphyton/ periphyton, zooplankton, macrophyte, CBOD, sediment diagenesis model and generic water quality groups.	Based on the algorithms developed by US Army Engineer Waterways Experiment Station (WES)in year 1975.	Open	Rivers, estuaries, lakes, reservoirs and river basin systems.	Water Quality Research Group of Portland State University, USA (http://www.ce.pdx.edu/w2/).
3	**EFDC** *(Environmental Fluid Dynamics Code)*	1D/2D/3D hydro-dynamic model for water and water quality constituent transport modeling	Salinity, temperature, suspended cohesive and non-cohesive sediment, dissolved and adsorbed contaminants, and a dye tracer.	It is a multifunctional surface water modeling system, which includes hydrodynamic, sediment-contaminant, and eutrophication components.	Developed by Dr. John M. Hamrick in year 1990 and subsequent support by the US-EPA.	Open	Rivers, lakes, reservoirs, wetlands, estuaries, and coastal ocean regions	Center for Exposure Assessment Models (CEAM), US-EPA
4	**HSCTM2D** *(Hydrodynamic, Sediment, and Contaminant Transport Model)*	2-D vertically-integrated, surface water flow sediment transport and contaminant transport.	Advection-dispersion of concentrations of suspended sediment dissolved and sorbed contaminants.	A finite element model. The modeling system consists of two modules, one for hydrodynamic modeling (HYDRO2D) and the other for sediment and contaminant transport modeling (CS2D). HYDRO2D solves the equations of motion and continuity for nodal depth-averaged horizontal velocity components and flow depths.CS2D solves the advection-dispersion equation for nodal vertically-integrated concentrations of suspended sediment, dissolved and sorbed contaminants, and bed surface elevations.	Developed by National Exposure Research Laboratory of the US-EPA in 1995.	Open	Riverine or estuarine hydrodynamics	Center for Exposure Assessment Models (CEAM), US-EPA

Sl. No.	Model	Dimensions and State of Hydraulics	Pollutant type it can handle	Description	Year of Development & by whom	Open /license	Applicability	Reference
5	**HSPF** *(Hydrological Simulation Program-Fortran)*	1-D stream channels and on watershed & basin scale.	It allows the integrated simulation of land and soil contaminant runoff processes with In-stream hydraulic and sediment-chemical interactions. It simulates water quality for both conventional and toxic organic pollutants.	HSPF incorporates watershed-scale ARM and NPS models into a basin-scale analysis framework that includes fate and transport in one dimensional stream channels.It simulates three sediment types (sand, silt, and clay) in addition to a single organic chemical and transformation products of that chemical.	Developed by the US EPA in year 1997	Open	Watersheds, Streams, and Lakes.	Center for Exposure Assessment Models (CEAM), US-EPA
6	**COASTOX**	2-D simulation of radionuclides in solute, suspended sediments and in bottom depositions of reservoirs, floodplains and coastal areas.	sediment transport, radionuclidetransports in shallow reservoir, ,lakes and coastal water	The model is used to analyze radionuclide dispersion in water bodies. It also calculates the dynamics of the bottom deposition contamination and describes the rate of sedimentation and resuspension.	Cybernetics Center, Kiev	-	Lakes, Reservoir & River	IAEA, Vienna
7	**WASP models** *(Water Quality Analysis Simulation Program)*	1D/2D/3D water quality simulation in rivers, lakes, estuaries, coastal wetland, and reservoirs.	Capable of handling multiple pollutant types including Total Maximum Daily Loads (TMDL).	WASP is a dynamic compartment-model for aquatic systems, including both water column and the underlying benthos. The time varying processes of advection, dispersion, point and diffuse mass loading and boundary exchange are represented in the model. It also can be linked with hydrodynamic and sediment transport models to provide flows, depths velocities, temperature, salinity and sediment fluxes. The latest release of WASP contains the inclusion of the sediment diagenesis model linked to the advanced Eutro-phication sub model to predict SOD and nutrient fluxes from the underlying sediments.	Developed originally by Di Toro *et al.*, in year 1983 and subsequently enhanced by Connolly and Winfield (1984); Ambrose, R.B. *et al.*, (1988)	Open	Rivers, Lakes, Estuaries, Coastal wetlands, and Reservoirs.	Center for Exposure Assessment Models (CEAM), US-EPA
8	**MIKE models** • MIKE 11 • MIKE 21 • MIKE31	1D/2D/3D unsteady	**MIKE 11 (1D):** DO, BOD, NO3, NH4, P, Coliform. MIKE 21 (2D): physical, chemical or biological processes in coastal or marine areas	**MIKE 11** simulates hydrology, hydraulics, water quality and sediment transport in estuaries, rivers, irrigation systems and other inland waters. **MIKE 21** simulates surface flow, waves, sediment transport and environmental processes and can be used for estuarine and coastal modeling. MIKE 31 for estuaries, coastal areas, and seas. It covers a wide range of	First developed in year 1995 and subsequently promoted by Denmark Hydrology Institute.	License	Rivers, Estuaries, and Tidal wetlands	DHI (https://www.dhigroup.com/)

Sl. No.	Model	Dimensions and State of Hydraulics	Pollutant type it can handle	Description	Year of Development & by whom	Open /license	Applicability	Reference
			MIKE 31 (3D): hydrodynamics, sediment dynamics, water quality and ecology.	hydrodynamic, environmental and sediment transport processes				
9	**DELFT3D**	3 D hydrodynamic Model	investigate hydrodynamics, sediment transport, morphology and water quality for fluvial, estuarine and coastal environments	The package consists of several modules coupled together to provide a complete picture of three-dimensional flow, surface waves, water quality, ecology, sediment transport and bottom morphology and is capable of handling the interaction between these processes.	Deltares	Open	Coastal waters, estuaries, rivers, lakes	Deltares (https://www.deltares.nl/en/)
10	**EUTROMOD** *(Eutrophication model)*	-	Nutrient loading, various trophic state concentration, and trihalomethane concentrations.	Watershed and lake modeling procedure for eutrophication management with emphasis on uncertainty.	Developed by Kenneth H. Reckhow in year 1992	License	Watershed& Lake.	North American Lake Management, Florida
11	**TSM** *(Lake Trophic Status Model)*	-	Mean Phosphorous concentration or values of other trophic status indicators, viz., chlorophyll a and Secchi depth.	It is based on empirical and semi-empirical equations. The model can include upto 15 tributary streams for study of a lake and upto 3 lakes upstream in each tributary.	Developed by Dillon and Rigler (1975)	Open	Lakes	Ontario Ministry of Environment, (1991).
12	**MINLAKE**	Dynamic 1 D model	Temperature, dissolved oxygen, phosphorus, Chlorophyl- a nitrogen and dissolved substances	Minlake model was developed to serve as a tool for evaluating lake management strategies. It include advective and diffusive transport, settling, chemical and biological kinetics.	Developed by Riley and Stefen (1987)	-	Lakes & Reservoirs	Riley and Stefen (1988)
13	**DYRESM 1D** *(Dynamic Reservoir simulation model)*	1D lagrangian hydro-dyamic model	Temperature, salinity and density in lakes and reservoirs	It provides a means of predicting seasonal and inter-annual variability of lakes and reservoirs as well as sensitivity testing to long-term changes in environmental factors or watershed properties	Center for Water Research, CWR, at the University of Western Australia	License	Lakes & Reservoir	Stolarska and Skrzypski (2012)
14	**ECM** *(Export Coefficient Model)*	-	Nutrient loading, Total N, Total-P	The ECM approach aims to predict the nutrient loading at any surface water sampling site as a function of export of nutrients from each contamination source in the catchment above that site. It relies on data from readily available databases. It is less data demanding model.	Developed in 1976 by J. M. Omernik of University of Reading, USA	Open	Watershed & River	Omernik, (1976)
15	**Dynamic River**		Simulates CBOD, DO,	Analyzes the impact of point source	Developed by US-	Computer		Yearsley, J.

Sl. No.	Model	Dimensions and State of Hydraulics	Pollutant type it can handle	Description	Year of Development & by whom	Open /license	Applicability	Reference
	Basin Water Quality Model	-	algal biomass, organic-N, NH_4-N, NO_2, NO_3, organic-P, orthophosphate, temperature, coliform bacteria, and two conservative constituents.	wastes from industries and municipalities, non-point sources and water diversion upon the aquatic ecosystems of freely-flowing rivers, river-run-reservoirs and stratified reservoirs.	Environmental Protection Agency (EPA) in year 1991.	Program is freely available.	Rivers & Reservoirs	(1991).
	CATCHMENT/WATERSHED WATER QUALITY MODEL							
16	**BASINS** *(Better Assessment Science Integrating point & Non-point Sources)*		BASINS assist in watershed management and TMDL estimation. It is a useful tool for watershed management, development of total maximum daily loads (TMDLs), coastal zone management, nonpoint source programs, water quality modeling,	BASINS is a multipurpose environmental analysis system model developed to help regional, state, and local agencies perform watershed- and water quality-based studies.	Developed by US-EPA	Open	Watershed	Center for Exposure Assessment Models (CEAM), US-EPA.
RIVER WATER QUALITY MODELS								
1	**CE-QUAL-RIV1**	1-D(longitudinal) Dynamic model	Temperature, DO, CBOD, Organic-N,NH_4-N, NO_3-N, Orthophosphate-P,Coliform bacteria, Dissolved Iron, Dissolved Mn, Algae and Macrophytes	Consists of two parts: a hydrodynamic (RIV1H) part, and water quality (RIV1Q) part. Model allows simulation in branched river systems with multiple hydraulic control structures and can simulate transient water quality conditions under unsteady state.	In year 1990 by US-Army Engineers Waterways Experiment Station.	Open	Rivers and Streams	Environmental Laboratory (1990)
2	**CHARIMA**	1-D fully mixed simulation model for unsteady mobile-bed hydrodynamics and contaminant transport modeling.	Mobile-bed sediment (bed load and/or suspended load) transport. Contaminant transport includes any number of conservative contaminants and heat.	CHARIMA model can simulate steady or unsteady water, sediment and contaminant transport in simple or complex systems of channels.	Iowa Institute of Hydraulic Research, University of Iowa, USA	Not available to outside users.	Rivers	Holly*et al.*, (1990)
3	**DSSAMT** *(Dynamic Stream and Simulation Model with Temperature)*	1-D Steady state river flow and 14 water quality constituents' model.	Water temperature, organic and inorganic fractions of nitrogen and phosphorous, BOD, DO, pH, alkalinity, CO_2, TDS, Chloride, blue green and non-blue-	The river processes the model considers include: equilibrium temperature and heat exchanges; advection, biochemical and physical kinetics of all 14 constituents including variation over 24-day; nutrient, spatial, and light limitation of benthic primary production; algal removal	Developed by Craig L. Caupp, James T. Brock, and Henry M. Runke from USA in year 1991.	The programme isavailable from Rapid Creek Research, Inc. Idaho, USA	Rivers	Rapid Creek Research, Inc. P.O. Box 2616;, Boise,Idaho, 83701-2616, USA.

Sl. No.	Model	Dimensions and State of Hydraulics	Pollutant type it can handle	Description	Year of Development & by whom	Open /license	Applicability	Reference
			green benthic algae, and coliform bacteria.	processes.				
4	**DRAINMOD**	-	Total N, salt	Developed to assist in the simulation of the transport of water and the transport and transformation of nitrogen in a stream. The most recent version of DRAINMOD PC version (released 6.1) has been extended to predict the movement of nitrogen (DRAINMOD-N) and salt (DRAINMOD-S) in shallow water table soils.	First developed in year 1980 and latest PC version in year 2012 by Soil & Water Management Group, North Carolina State University, USA	Open	Drain, Stream and Soil.	Skaggs, (1981)
5	**DUFLOW 1D**	1D unsteady flow for open watercourses.		A micro-computer package for the simulation of one-dimensional unsteady flow and water quality in open channel systems	International Institute for Hydraulic and Environmental Engineering (IHE) The Netherland,	A free student's version is available, which includes all options, but is restricted in the number of channel sections and structures.	Open Channel, Rivers	IHE, TU Delft, Wageningen University and Stowa
6	**SIMCAT** *(Simulation of Catchments)*	1-Dimensional, deterministic, steady state.	Determines fate and transport of solutes in rivers from point sources, particularly DO, BOD, NO_3 and conservative substances.	It is a stochastic model and makes use of Monte Carlo analysis technique. The model helps in the process of planning the measures needed to improve water quality in a catchment. The model can account for 600 reaches and 1400 features such as discharges and abstractions. SIMCAT ver. 6.0 can be used for Integrated water quality modeling.	Developed by Scottish Environmental Protection Agency.	Open	River	Warn, A. E. (1987)
7	**STREAMDO-IV** *(Stream Dissolved Oxygen Model)*	1-Dimensional steady state model	DO and Unionized NH_4.	It is a spreadsheet based model for analyses of waste load in river reaches. It requires flow, velocity, slope, depth, temperature, DO, CBOD, organic nitrogen, ammonia, nitrite, nitrate, pH, and SOD as inputs.	Developed by US-EPA in 1990.	Open	River	Zander and Love, (1990)
8	**Streeter-Phelps (S-P) models**	1-Dimensionalsteady-state& Mechanistic	BOD and DO	S-P models focus on oxygen balance and 1st order decay of BOD.	First established by Streeter-Phelpsin year 1925, thereafter modified by O'Connor, Dobbins-Camp	Open	River	Streeter and Phelps (1925)
9	**TOMCAT**	1-Dimensional	DO, NH_4, BOD	The model uses Monte Carlo analysis technique to review the effluent quality	Developed in year 1984	-	River	Bowden and

Sl. No.	Model	Dimensions and State of Hydraulics	Pollutant type it can handle	Description	Year of Development & by whom	Open /license	Applicability	Reference
	(Temporal/Overall Model for Catchment)	steady state (time invariant)		standards at sampling sites to meet the objectives of surface water quality preservation. The model allows complex temporal correlations taking into account the seasonal and diurnal effects in the flow data and the recorded water quality and reproduces these effects in the simulated data. TOMCAT calculates quality and flow in each reach by solving the process equations.	by Bowden and Brown,			Brown, (1984)
10	**QUAL models** • **QUAL I** • **QUAL II** • **QUAL2E** • **QUAL2E-UNCAS** • **QUAL 2K** • **QUAL2Kw**	1-Dimensional steady-state or dynamic model	It can simulate 15 water quality constituents in a branching stream system, viz. Total-N, Total-P, BOD, DO,NH_4 –N, NO_2-N, NO_3-N, SOD, algae, pH, periphyton pathogen.	The model uses finite difference solution of the advective-dispersive mass transport and reaction equations. The model simulates changes in flow conditions along the stream by computing a series of steady-state water surface profiles and the calculated stream-flow rate, velocity, cross-sectional area, and water depth serve as a basis for determining the heat and mass fluxes into and out of each computational element due to flow. QUAL2E uses chlorophyll a as the indicator of planktonic algae biomass. QUAL2E-UNCAS includes uncertainty analysis of using Monte Carlo simulation (MCS) of constituents.	QUAL I was developed by the Texas Water Development Board in year 1960.Thereafter, several improved versions of the model were developed by US-EPA. Last release was Jan., 2009.	Open	River	CEAM of US-EPA
11	**QUASAR model**	1-Dimensional dynamic model.	Simulates 8 variables in additional to flow; NO_3, ionized and unionized NH_4, DO, BOD, pH, temperature and any conservative or inert material in solution.	The river system is modelled by a series of reaches. The model performs a mass balance of flow and quality of each reach taking into account inputs from previous reach, tributaries, effluent discharges and abstractions.	Developed by the Institute of Hydrology, UK in year 1997.	Open	Large river	Center for Ecology and Hydrology,UK (http://www.ceh.ac.uk/services/pc-quasar)

The models like, HSCTM2D, DELFT3D and Dynamic River Basin have found their limited applications in water quality modeling. The Dynamic River Basin water quality model is available free of cost from their developers and can further be explored as it has capability to simulate a number of water quality parameters.

The listed 11 water quality models (Table 5.2) developed specifically for river water quality modeling also showed a mixed acceptability. The CHARIMA model, which is license based, has not been widely used outside USA. Similarly, the DSSAMT model, though capable of simulating most of the water quality conditions in a river system where polluting substances enter the modelled reach from a variety of sources, including tributaries, point effluent discharges, surface water point and non-point runoff, groundwater, leaching and scouring from the bottom sediments, however has find limited applications. The DRAINMOD, DUFLOW 1D and STREAMDO-IV models have their limited applicability with limiting modeling capabilities. The models like CE-QUAL-RIV1, SIMCAT, TOMCAT, Streeter-Phelps (S-P) models, QUAL series models (i.e., QUAL I, QUAL II, QUAL2E, QUAL2E- UNCAS, QUAL 2K) and QUASAR model have been widely used for water quality modeling. Cox (2003), Jha et al. (2007), Gao and Li (2014), Kannel et al. (2011) discussed the modeling capabilities and limitations of some of these models. The most used models by the UK Environment Agency are SIMCAT and TOMCAT, however, they rarely appeared in the literature (Jamieson and Fedra, 1996), because they are not generally used for regulation outside of the UK and this is probably due to their stochastic component as well as a lack of commercial exposure.

Majority of water quality professionals refer to the United States Environmental Protection Agency (USEPA) model QUAL2E, with reported applications in the Americas, Europe, Asia and Australasia (Cox, 2003). The QUAL2E model is probably the most widely-used water-quality model in the world and although it is unable to handle temporal variability in a river system. The QUAL2E was first released in 1985 and the USEPA has used and improved this model extensively since then. More recently, the model has been integrated with other USEPA models such as, HSPF and WASP in a GIS (Geographical Information System) environment in software called BASINS. Thus, QUAL series of the models is more comprehensive and has worldwide acceptability and applicability than the other models. The QUAL2E is a much more complex model than SIMCAT and TOMCAT models. QUAL2E is the latest version of QUAL-II and has been wildly used in water quality prediction and pollution management (Gao and Li, 2014). Zhang et al. (2012) showed that QUAL2K is an effective tool for the comparative evaluation of potential water quality improvement programs through simulating the effects of a range of water quality improvement scenarios. The main advantage of QUAL2K is the capability of simulation of algae (Chlorophyll-a), an extensive documentation of its code and theoretical background. An extension of the QUAL2E model called QUAL2E–UNCAS allows the user to perform uncertainty analyses by investigating model sensitivity to changes in one variable at a time (sensitivity analysis) or all of the variables at once (first-order error analysis) or by using Monte Carlo techniques. The QUASAR is well suited to investigating lowland river systems. Sharma and Kansal (2013) found that the models namely, QUAL2Kw, WASP and AQUATOX are capable of simulating maximum number of parameters. AQUATOX, QUAL2Kw and WASP include the sediment diagnosis model for re-mineralization. QUAL2Kw can also simulate SOD and hyporheic metabolism, which are vital for predicting river water quality and for planning the management options. As observed, WASP model has an advantage of simulating toxicants as well. Therefore, looking into the overall applicability and simplicity of the models, and their availability, the following models are finally short-listed (Table 5.3) for direct applications or their inter-coupling and interfacing to provide most sustainable solution to water quality assessment and management problems.

5.8 Ways Forward

Surface water quality management is a critical component of overall integrated water resources management. Water quality modeling as a powerful tool can give answers to a large number of management questions related to prospective social, economic, environmental, technical and political issues of future scenarios based on past and present conditions. Decisive use of water quality modeling in India as a tool for policy evaluation & decision, water quality management, risk assessment, and water quality conservation is yet to pick up momentum in India. Some of the reasons behind this are; (i) inadequate spatio-temporal water quality data to conceive, calibrate and validate a model, (ii) lack of information/data on source of pollution and their magnitude and characteristics, (iii) inadequate data and understanding on water quality hydrodynamics and kinetics to describe the physical behaviour of the water systems, etc. Growing concern on drinking water security, emerging threat to ecosystem and environmental imbalances, and climate change impacts on water quality together with population pressure for safe and sustainable water quality, pose major challenges to maintaining sustainability in water quality management. Organized surface water quality monitoring networks together with increased frequency of monitoring can help build good databases for adoption of large-scale water quality modeling approach in policy planning, evaluation and decision, management of river and other surface water quality conservation and management, etc. of India. Generation of good water quality databases including contaminant kinetics is one of the primary requirements; on the other hand, systematic and continual capacity building on water quality modeling is another important pursuit the nation should adopt for resolving water crisis emerging from water quality threat. The report has brought out a comprehensive list of surface water quality models developed and successfully adopted for solving different environmental and water quality problems world over. Some of those models are generic, process based, less data driven and have proven effective and capable to simulate conditions prevalent in India. It is, therefore, desirable that the potential of adopting some of those models, which have open access, be studied in detailed with the understanding of India's water system's hydro-physicochemical & biological conditions, instead of developing per se new version of surface water quality models. The pursuit should also be focused towards integrating the modules developed based on the study of India's hydro-physicochemical & biological conditions, with the existing models. Amongst the potential water quality models, HSPF for watershed, streams, and lakes; WASP 7 for rivers, lakes, estuaries, coastal wetlands, and reservoirs; and QUAL series for rivers and streams, developed and promoted by US-EPA (all have open access) are found most promising for detailed study, and recommended for inclusion as an integral part of the comprehensive hydrologic model that the Institute is focusing under the National Hydrology Project.

Table 5.3 Selected Water Quality Models based on their Applicability, Modeling Capability, Availability and Processes Involved

Models		AQUATOX	HSPF	CE-QUAL-W2	WASP7	EFDC	QUAL Series		MIKE Series
							QUAL2E-UNCAS	QUAL 2KW	
Types (Dimension and State of Hydraulics)	1D	N	Y	N	Y	Y	1D	Y	Y
	2D	Y	N	Y	Y	Y	N	N	Y
	3D	N	N	N	Y	Y	N	N	Y
	Steady state	Y	N	N	N	N	Y	Y	N
	Dynamic	Y	Y	Y	Y	Y	Y	Y	Y
	Stochastic	Y	N	N	N	N	N	N	N
Modeling Approach	ADE	N	N	Y	Y	Y	Y	Y	Y
	CSTRS	Y	Y	N	N	N	N	N	N
Modeling capability	Temp., Bacteria, DO-BOD, Nitrogen Phosphorous Silicon Phytoplankton Zooplankton Benthic algae SOD, COD CBOD Sediment, etc)	pH, DO nutrients, NH4 toxicity, detritus, Phytoplanton, Periphyton, Zooplankton, sediment digenesis, fish, invertebrates, and aquatic plants	pH, NH4, DO, BOD, temp., pesticides,conservatives, fecal coliforms,sediment detachment and transport, nitrite-nitrate, organic nitrogen, orthophosphate, organic Phosphorous, phytoplankton, and zooplankton.	Nutrients, DO, organic matter interactions, fish habitat, multiple algae, epiphyton/periphyton, zooplankton, macrophyte, CBOD, TOC, sediment diagenesis, and generic water quality groups	DO, temp, N (ON, NO2, NO3 NH3), P (OP, PO4), coliform, salinity, SOD, CBOD, bottom algae, silica, pesticides, OCHEM	Salinity, temp.,suspended cohesive and non-cohesive sediment, dissolved and adsorbed contaminants, and dye tracer	Temp., Chlorophyll-*a* Bacteria, DO-BOD, N, P, Silicon, Phytoplankton Zooplankton Benthic algae, uncertainity analysis	Temp, pH, N (ON, NO2, NO3 NH3), P (OP, PO4), DO, CBOD, TIC, alkalinity, phytoplankton, bottom-algae, SOD, detritus, pathogen	Temp. Bacteria DO-BOD Nitrogen Phosphorus Silicon Phytoplankton Zooplankton Benthic algae
Availability (Open /license)		Open	Open	Open	Open	Open	Open	Open	License
Applicability		Lakes and reservoirs	Watersheds, Streams, and Lakes	rivers, estuaries, lakes, reservoirs and river basin system	Rivers, Lakes, Estuaries, Coastal wetlands, and Reservoirs	Rivers, lakes, reservoirs, wetlands, estuaries, coastal ocean regions	Rivers and streams	Rivers and streams	Rivers, Estuaries, and Tidal wetlands
Source/Reference		Center for Exposure Assessment Models (CEAM), US-EPA.		Water Quality Research Group of Portland State University, USA.	Center for Exposure Assessment Models (CEAM), US-EPA.		Center for Exposure Assessment Models (CEAM), US-EPA		DHI

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