

WORKSHOP
ON
MODELLING OF HYDROLOGIC SYSTEMS

4-8 September, 2000

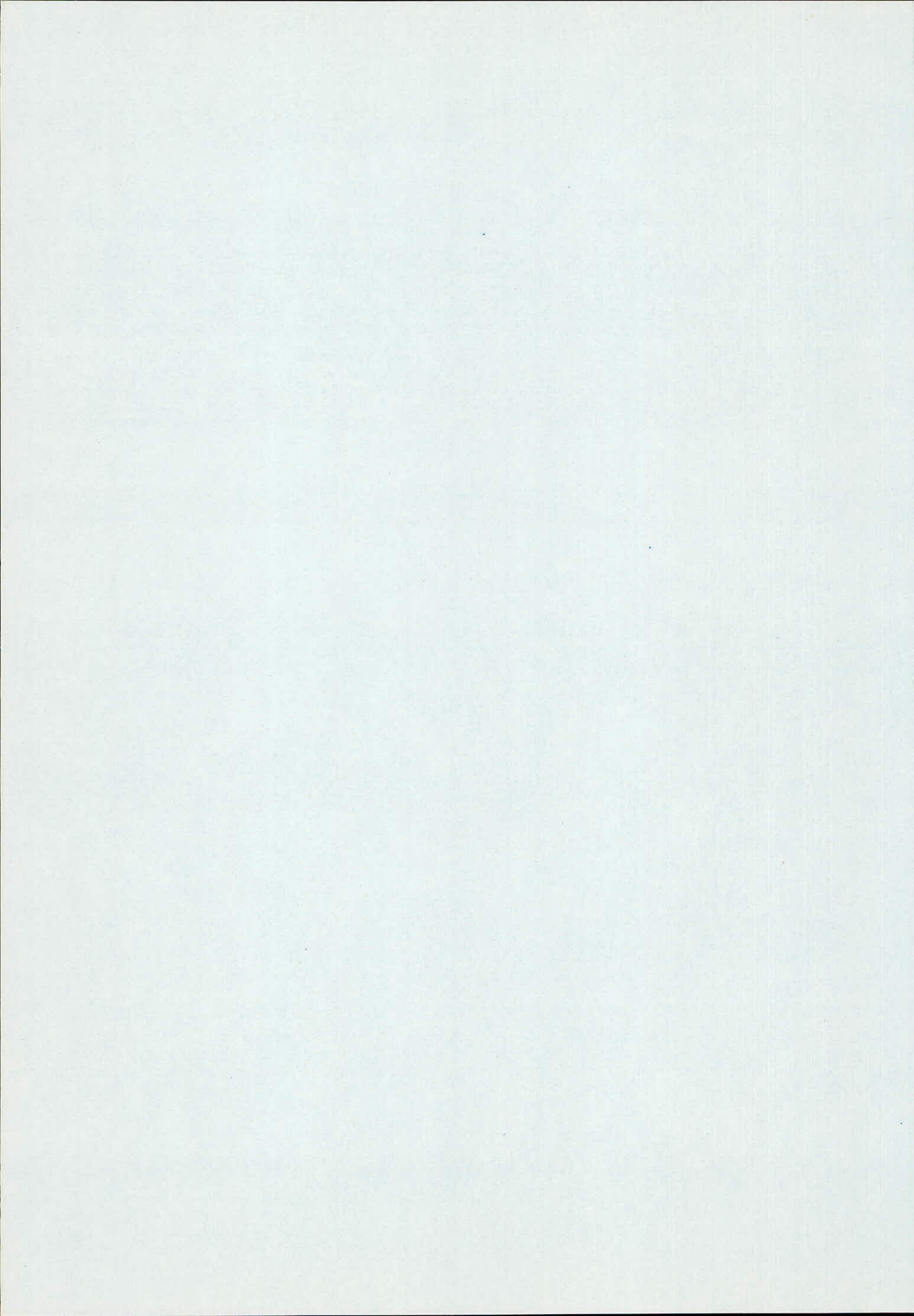
Water Quality Modelling (QUAL2E)

by
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1.0 Introduction

The environmental consequences of industrialization and intensification of agriculture have, for a long time, been neglected and unfortunately still are in many parts of the world. Exploitation of mineral resources and energy production have made deep cuts into the natural landscape and altered the flow of water in large river basins. Concentrated effluents from manufacturing and industrial production plants have added hazardous substances to natural watercourses and reduced their ability to sustain aquatic life. The rapid increase in population density has generated human wastes, which have reached surface waters or percolated into the ground with both immediate contamination and long term deterioration of the aquatic environment. To feed the ever-increasing populations a highly intensified agoro-industry, depending more on massive use of chemicals as fertilizers or pesticides, has emerged in the industrialized as well as many developing countries like our country.

Water is one of the factors required to boost crop yield and this has led to water demands which amount to three-quarters of all fresh water used on the globe. Competition among water users and costly investments to defend and maintain water quality at acceptable levels have been the inevitable consequences. The latter is particularly troubling relatively the economy of the country especially those situated in the arid and semi-arid climatic zones.

Problems with water contamination are, unfortunately not limited to single watersheds but cover great areas within and between continents. The recent realization that the mobility and chemical activity of water in the atmosphere, and in terrestrial branches range transport of pollutants was perhaps surprising. Anthropogenic activities in one place are the cause of water quality deterioration and ecological disturbances elsewhere (Falkenmark et al. 1987). The sulphur imports from other European countries is an example of this phenomena (Peterson et al. 1987). Deteriorating forest are another consequences of long range atmospheric transport of air pollution which also poses an increasing threat to surface and ground water resources. Pesticides are also becoming widely dispersed within the environment and, owing to their environmental mobility and persistence over long periods of time, are found in aquatic ecosystem either accidentally through spray drift, agricultural run-off and transport or deposition of airborne pesticides and precipitation, or are introduced as a means of controlling aquatic pests or even knowingly discharged with industrial effluents from production plants (Chapman, 1987). As a consequence, environmentalists are concerned about the cost of long time damage which at least in part, oxides the benefits gained from large-scale use of pesticides in agricultural production.

1.1 Water quality Assessment

The need of the water quality assessment attempts to answer the following questions

- i) What is the state of water quality on a global scale and in our country.
- ii) Impact of industrialization and modernization in agriculture sector on water quality.
- iii) Role of water quality managers in planning and management
- iv) Research needs in water quality
- v) Role of society in maintaining the environment.

Many of these questions require immediate attention from the society, scientists and politicians. Human activities and biogeochemical processes in other environmental compartments play a crucial role in determining what happens in watercourses and to aquatic biota.

1.2 Water Quality Modeling

Any rational formulation of water pollution control policies and programs cannot be possible without adequate knowledge of the existing nature, magnitude and sources of the various pollution loads which degrades the quality of river water. The study of behavior of these pollution loads specially the concentration profile of different pollutants in the river water is equally important to assess the degree of pollution that are prevailing and to identify the stretches which violate the standards and harmful for use over and above to determine the permissible assimilative capacity of the river, it is necessary to assess the prevailing status of pollution and their probable trends.

For preparing a realistic pollution control programme one should not only have a current inventory of pollution loads and the quantity and quality of water in various water bodies. For during this, it would be necessary to analyze and develop interrelationship between various aspects of human activities, stream flows, pollution loads and water quality.

1.2.1 Why Model ?

In modern life, modeling has become common practice in almost every field of endeavor, and water quality analysis and planning is no exception. The ultimate value of models of any kind is two fold: first to understand and reproduce how the modeled system works, and then to predict how the system will respond to future alternative conditions and actions. Within a watershed, the water quality at any location is determined by the net contributions from all point and non-point sources. Evaluating the net effect that can be expected from implementing one or more actions within the watershed is not at all straightforward. For example, contour plowing of agricultural lands may reduce the surface runoff of nitrates from fertilizer, but at the same time may result in increased nitrate percolation in subsurface flows, and subsequent threat to drinking water supplies derived from wells. Hence reliance on intuition, engineering experience and/or simplified analysis techniques is not an appropriate means for making management decisions that can have extreme economic and environmental consequences. The need to consider the full breadth of processes that determine the fate and transport of water driven materials has given rise

to the current popularity of the term 'comprehensive water quality analysis'. As a rule, truly comprehensive analysis cannot be achieved without the use of complex mathematical models.

Introductions to modeling and modeling caveats have been presented by several authors including James and Burges (1982), Kibler (1982), Huber(1985, 1986), Donigian and Huber (1991), and EMWG (Exposure Modeling Work Group of the National Agricultural Chemicals Association) (1994); additional summaries have been provided in at least one manual of practice (WPCF, 1989), as well as the Federal Register (EPA, 1992b). While space does not permit a full discussion of the necessary activities for successful model applications, a few fundamentals are highlighted sequentially below.

1. Have a clear statement of project objectives. Verify the need for quality
2. modeling.(Perhaps objectives can be satisfied without modelling).
3. Identify the processes that govern chemical behavior.
4. Formulate questions to be answered and scenarios to address them.
5. Establish constraints (time frame, costs, technology, availability and accuracy of data)
6. Assess the required level of sophistication.
7. Identify and evaluate candidate models.
8. Select appropriate model. Use the simplest model that will satisfy the project objectives. Often a screening model, e.g., regression or statistical, can determine whether more complex simulation models are needed. To the extent possible, utilize a quality prediction method consistent with available data.
9. Only predict the quality parameters of interest and only over a suitable time scale. Seasonal or annual loads will sometimes be all that is required.
10. Perform a sensitivity analysis on the selected model and familiarize with the model characteristics.
11. Calibrate and verify the model results. Use one set of data for model calibration and another for verification.
12. Apply model to answer the questions.
- 12 Reduce results; perform visualization and statistical analysis. Assure quality assurance /quality control.
13. Implement management strategies based on model results; educate managers or regulators on appropriate modeling caveats.

Proper model applications account for relevant governing processes at an appropriate detail (time step and spatial scale) and accuracy relative to, achieving the objectives of the study. The level of sophistication required in a modelling study reflects constraints such as:(1)accuracy required , (2) allotted time frames, (3) current technology in describing environmental fate behavior and (4) availability and reliability of input data. These constraints dictate model selection, whether modeling is an appropriate tool for achieving the objectives, and the limitations in interpreting the model results. Model selection should also consider the availability of pre- and post processors which are designed to facilitate model setup and interpretation of results, quality and organization of model documentation, and availability of user support. Significantly managers and regulatory officials must be educated on assumptions and limitations associated with interpreting the results of a modeling study.

Confidence in model results is based on the quality of data used to construct the model, the capabilities of the modeler, and the proven ability of the to simulate observed phenomena(EMWG, 1994).

1.2.2 Role of Modeling in Water Quality analysis

The fate of chemicals in the environment is determined by the complex interaction of numerous factors including: physical and chemical properties of the chemical; the natural occurrence or application practices associated with the chemical; the characteristics of the surface and subsurface media through which transport occurs; and climatological conditions. In a similar manner, sediment fate and transport is affected soils properties, topography, weather and man-induced disturbances and controls.

Simulation models provide a mechanism to evaluate these interactions and estimate the extent the chemicals may move to non-target environments, such as surface receiving waters or groundwater aquifers. Further, modelling allows such evaluations to be performed in a time - and cost effective manner when compared to conducting resource intensive field monitoring studies. Generally, a high degree of confidence is associated with the results of a field study, because field studies are not practical in all cases. The results of the field study represent only one specific location under one set of environmental conditions. In contrast, simulation model permit the relative impacts of numerous environmental parameters to be evaluated. Since simulation models are mathematical representations of physical, chemical and biological processes, confidence in model results reflect the degree and the proven ability of the model to reproduce observed phenomena.

1.3 QUAL2E Model

QUAL2E, is a comprehensive and versatile stream water quality model, permits simulation upto 15 water quality constituents in any combination desired by the user in a branching stream system using finite difference solution to the one-dimensional advective dispersive mass, transport and reaction equation.

Constituents who can be simulated are

- (i) Dissolved Oxygen
- ii) Biochemical Oxygen Demand
- iii) Temperature
- iv) Algae as Chlorophyll
- (v) Organic Nitrogen as N
- (vi) Ammonia as N
- (vii) Nitrite as N
- (viii) Nitrate as N
- (ix) Organic Phosphorous as P
- (x) Dissolved Phosphorous as P
- (xi) Coliforms

- (xii) Arbitrary Nonconservative Constituent
- (xiii) Three Conservative Constituents

The model allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow. It also has the capability to compute required dilution flows for flow augmentation to meet pre-specified dissolved oxygen level. The model can either be used as a steady state or as dynamic model. When operated as a steady-state model, it can be used to study the impact of waste loads (magnitude, quality and location) on in stream water quality and also can be used in conjunction with a field sampling program to identify the magnitude and quality characteristics of non-point source waste loads. By operating the model dynamically, it is possible to study the effects of diurnal variations in meteorological data on water quality (primarily dissolved oxygen and temperature) and also can study diurnal dissolved oxygen forcing functions, such as headwater flows or point loads, cannot be modeled in QUAL2E.

QUAL2E-Uncas is enhancement to QUAL2E, which allows to perform uncertainty analysis on the steady state water quality simulations. Three uncertainty options are available: Sensitivity analysis, first order error analysis, and monte-carlo simulations. With this analysis, the effect of model sensitivities and of uncertain input data can forecast. Quantification of the uncertainty in model forecasts allows assessment of the risk (probability) of a water quality variable whether above or below an acceptable level. The uncertainty methodologies provide the means whereby variance estimates and uncertainty prediction can become as much a part of water quality modelling as estimating expected values is today. An evaluation of the input factors that contribute most to the level of uncertainty will lead in the direction of most efficient data gathering and research. In this manner it is possible to assess the risk of imprecise forecasts, and recommended measures for reducing the magnitude of that imprecision.

1.3.1 Model Representation and Limitations

QUAL2E permits simulation of any branching, one-dimensional stream system. The first step in modeling a system is to sub-divide the stream system into reaches. Each reach is then to be divided into computational elements of equal length to represent an integer number of equal computational elements(fig 1).

1.3.2 Concepts in Formulation of Model

The primary objective of any stream water quality model developemnt is to produce a tool that has the capability for simulation the behavior of the hydrologic and water quality components of a stream. QUAL2E has also been developed to simulate prototype behavior by applying sets of mathematical equations as applicable for water quality simulations. Three general phases (Water Resources Engineers, Inch, 1967) have been considered for formulation of the model:

- (i) Conceptual Representation
- (ii) Functional Representation
- (iii) Computational Representation

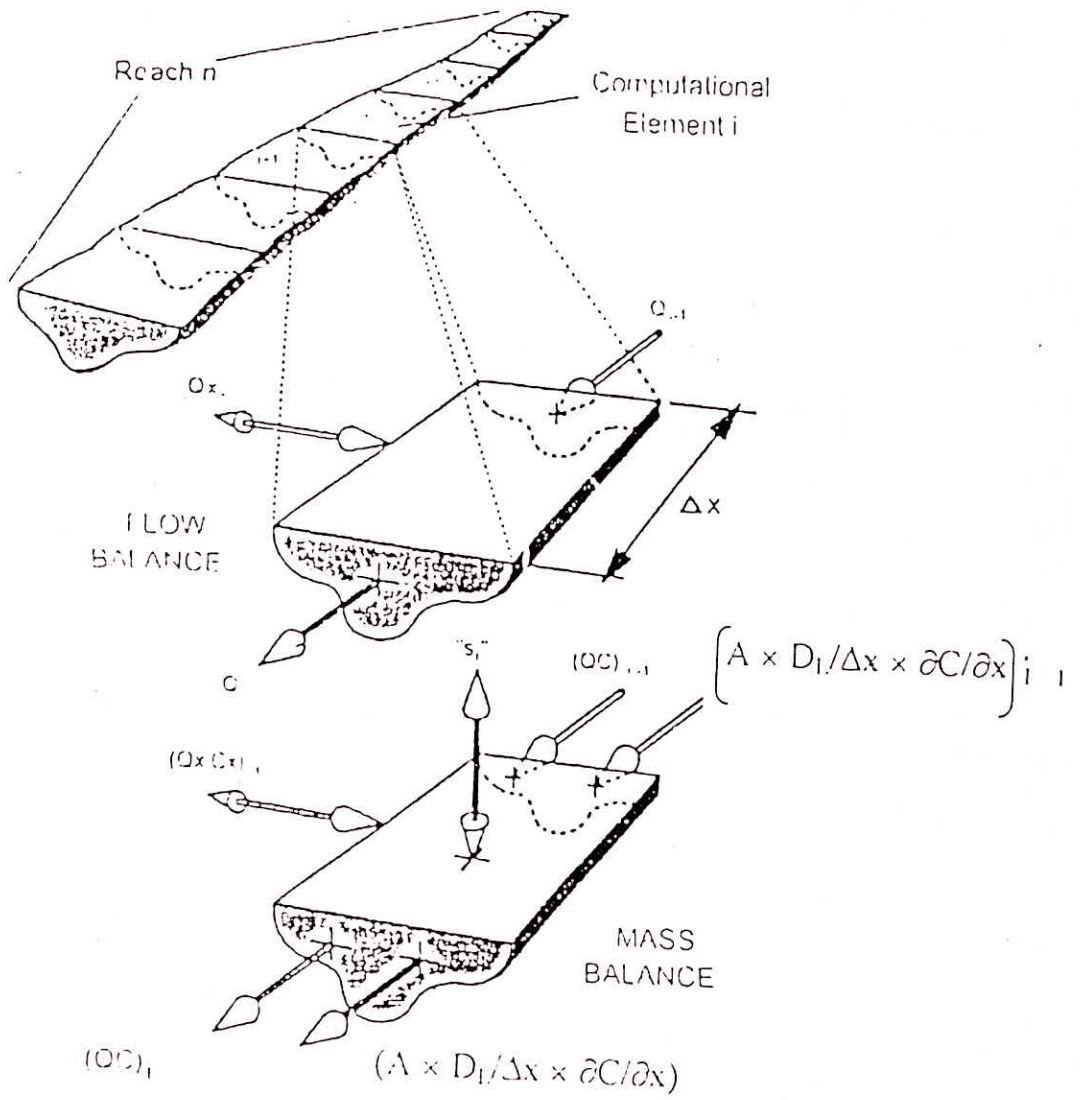


Fig. 1. Conceptual Representation of QUAL2E Discretized Stream System

(i) Conceptual Representation

Conceptual representation involves a graphic idealization of the prototype by description of the geometric properties that are to be modeled and by identification of boundary conditions and interrelations between various parts of prototype relations. Fig 2 shows a stream reach (n) that has been divided into a number of subreaches or computational elements, each, of length Δx . For each of these computational elements, the hydrologic balance in terms of inflows into the upstream face of the element (Q_{i-1}), external sources or withdrawals (Q_{xi}), and the flow (q_i) through the downstream face of the element has been written. In the similar fashion, a materials balance for any constituent C is written for the element. In the material balance, both transport ($Q.C$) and dispersion ($A \times (D_{si} / \Delta x) \times (\partial C / \partial x)$) as the movers of mass along the stream axis has been considered. Mass can be added to or removed from the system via external sources and withdrawals ($Q_x C_x$), and added or removed via internal sources or sinks (S_i) such as benthic sources and biological transformation. Each computational element is considered to be completely mixed.

(ii) Functional Representation

The basic equation that has been solved in formulation of QUAL2E is the one-dimensional advection-dispersion mass transport equation, which has numerically been integrated over time and space for each water quality constituent. This equation includes the effects of advection, dispersion, dilution, constituent reactions and interactions, and sources and sinks. For any constituent C, this equation can be represented as

$$\frac{\partial M}{\partial t} = \frac{\partial \left(A_x D_L \frac{\partial C}{\partial x} \right)}{\partial x} dx - \frac{\partial \left(A_x u C \right)}{\partial x} + \left(A_x dx \right) \frac{dC}{dt} + S \dots\dots\dots(1)$$

where

- M = mass (M)
- X = distance (L)
- T = time(T)
- C = concentration (ML⁻³)
- A_x = cross sectional area (L²)
- D_L = dispersion co-efficient (L²T⁻¹)
- U = mean velocity (L T⁻¹)
- S = external source / sinks (MT⁻¹)

Because, M = V.C and V= A_x dx. Assuming flow in the stream is steady, i.e. $\partial Q / \partial t = 0$, then

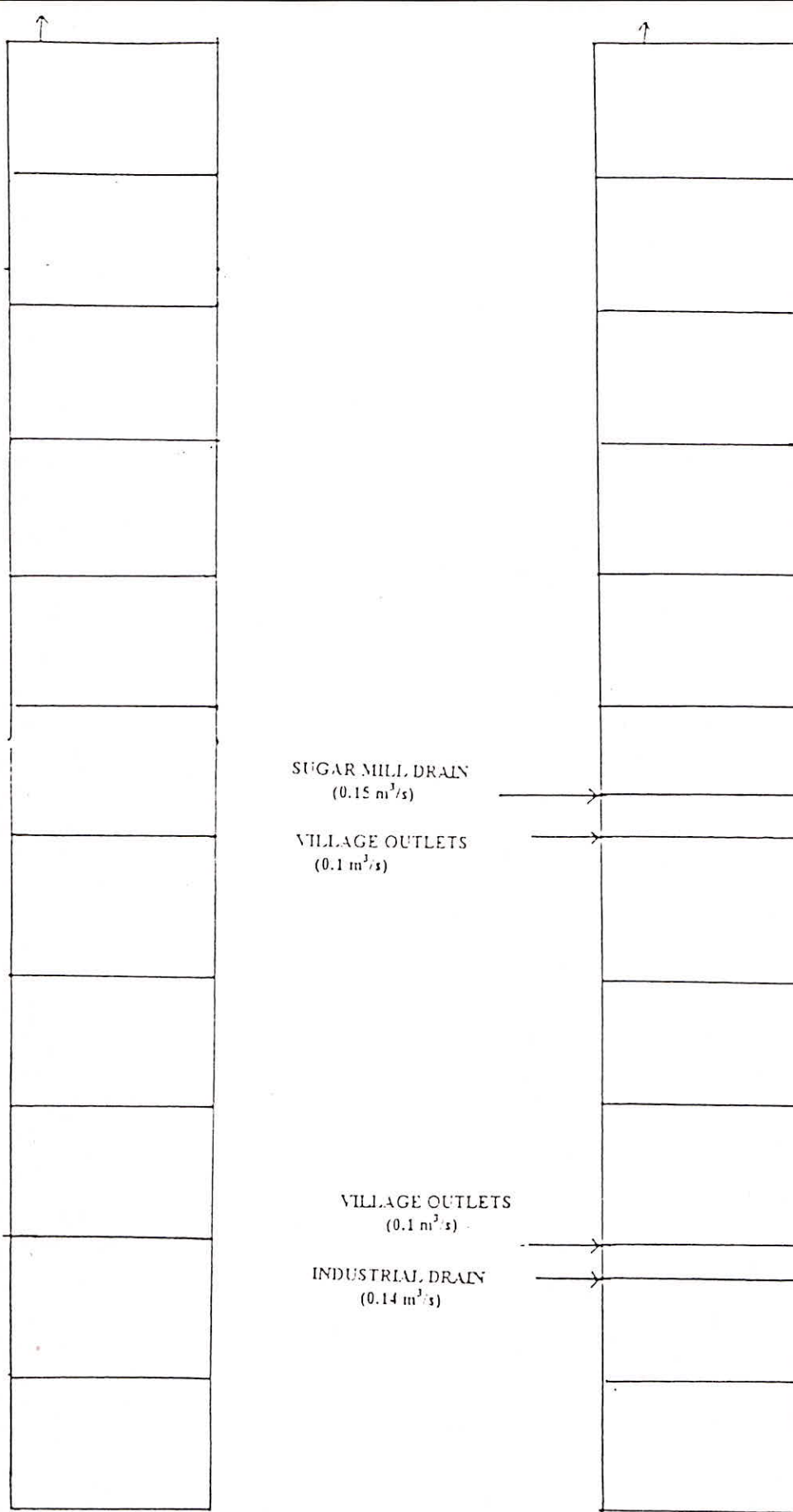


Fig. 2. Discretization of study stretch

$$\frac{\partial C}{\partial t} = \frac{\partial \left(A D_L \frac{\partial C}{\partial x} \right)}{A \frac{\partial x}{\partial t}} - \frac{\partial \left(A u C \right)}{A \frac{\partial x}{\partial t}} + \frac{S}{V} \dots \dots \dots (2)$$

The terms on the right hand side of the equation represent respectively,, dispersion, advection, constituent changes, external sources/sinks, and dilution. The dC/dt term refers only to constituent changes such as growth and decay, $\partial C / \partial t$ on the left-hand side is the local concentration gradient. The later term includes the effect of constituent changes as well as dispersion, advection, sources/sinks, and dilutions.

Under steady-state conditions, the local derivative becomes equal to zero; i.e.,

$$\frac{\partial C}{\partial t} = 0 \dots \dots \dots (3)$$

Changes that occur to individual constituents or particles independent of advection, dispersion and waste inputs are defined by the term;

$$\frac{\partial C}{\partial t} = 0 \dots \dots \dots (4)$$

These changes include the physical, chemical and biological reactions and interactions that occur in the stream.

1.4 Constituent Reactions and Interrelationships

One of the most important considerations in determining the waste assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. Dissolved oxygen concentrations in stream are controlled by atmospheric reaeration, photosynthesis, plant and animal, respiration, benthic demand, BOD(Bio-chemical Oxygen Demand), nitrification, salinity and temperature, among, other factors.

The QUAL2E model (fig 3) includes the major interactions of the nutrient cycles, algae production, benthic oxygen demand, carbonaceous oxygen uptake, atmospheric aeration and their effect on the behavior of dissolved oxygen. Fig. () indicates the conceptualisation of major constituent interactions considered in QUAL2E.

The mathematical relationships of parameters that have been considered in QUAL2E and are of interest have been outlined below

1.4.1 Dissolved Oxygen

Considering the interactions and reactions in oxygen balance as indicated in the differential equation for DO assumed in QUAL2E is given below:

$$(dO/dt) = K_2 (O^*-O) + (\alpha_3\mu - \alpha_4 \rho) A - K_1L - (K_4/d) - \alpha_5\beta_1N_1 - \alpha_6\beta_2N_2) \dots \dots 5$$

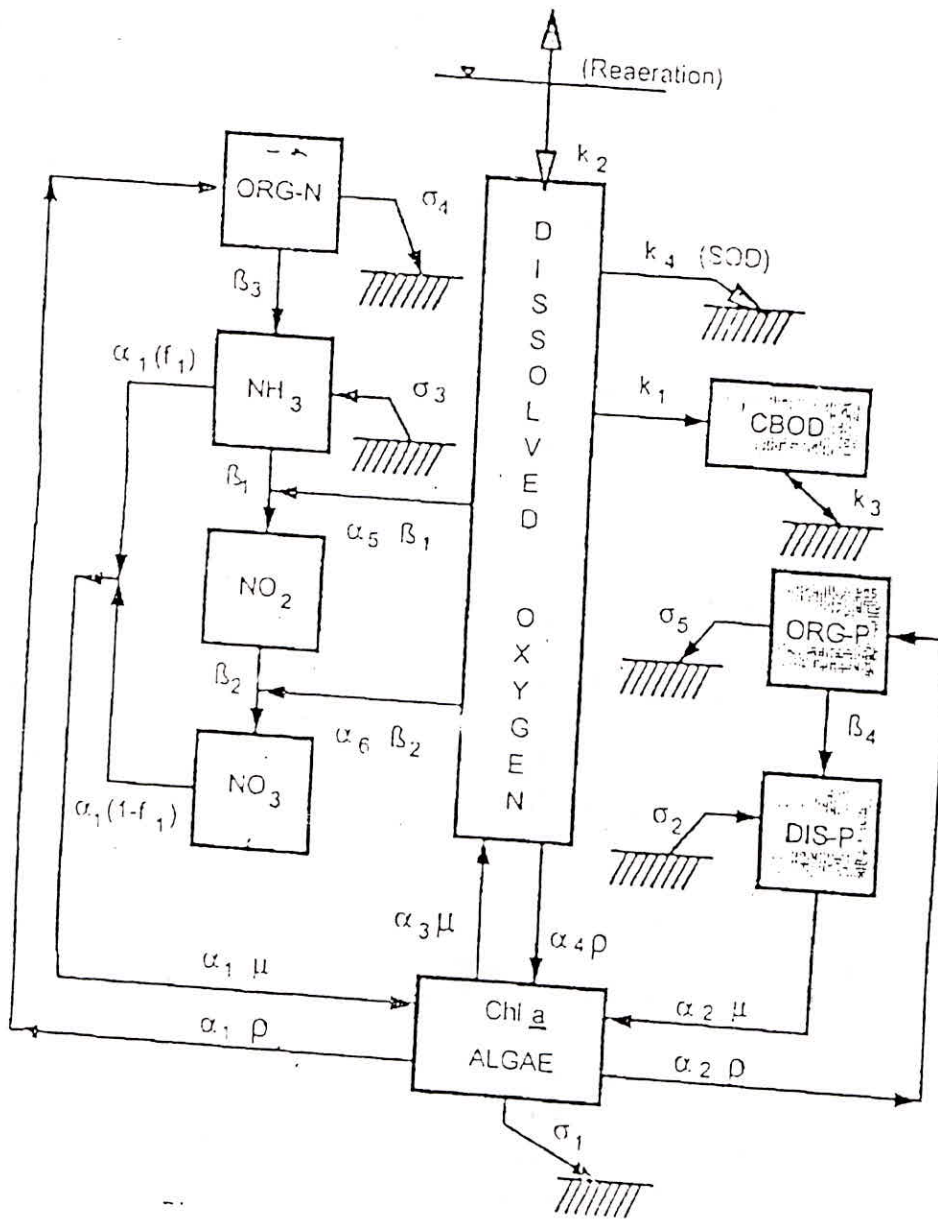


Fig. 3 QUAL2E Constituent Schematic for DO Simulation

where,

- O = concentration of dissolved oxygen (mg/l)
 O* = the saturation concentration of dissolved oxygen at the local temperature and pressure, (mg/l)
 α_3 = the rate of oxygen production per unit of algal photosynthesis, (mg/O /mg-A)
 α_4 = rate of oxygen uptake per unit of algal respired (mg-O / mg-A)
 α_5 = rate of oxygen uptake per unit ammonia nitrogen oxidation (mg-O / mg -N)
 α_6 = rate of oxygen uptake per unit of nitrite nitrogen oxidation, (mg-O/mg-N)
 μ = algal growth rate, temperature dependent , (per day)
 ρ = algal respiration rate, temperature dependent, (per day)
 A = algal biomass concentration (mg-A /l)
 L = Concentration of ultimate carbonaceous BOD(mg/l)
 d = mean stream depth
 K_1 = carbonaceous BOD deoxygenating rate, temperature dependent (per day)
 K_2 = the reaeration rate in accordance with the Fickian diffusion analogy, temperature dependent (per day)
 K_4 = sediment oxygen demand rate, temperature dependent, (g/ft^2 per day)
 β_1 = ammonia oxidation rate coefficient, temperature dependent (per day)
 N_1 = ammonia nitrogen concentration (mg- N/l)
 β_2 = nitrite oxidation rate coefficient, temperature dependent (per day)
 N_2 = nitrite nitrogen concentration (mg - N /l)

1.4.2 Dissolved Oxygen Saturation Concentration

The solubility of dissolved oxygen in water decreases with increasing temperature, increasing dissolved solid concentration and decreasing atmospheric pressure. QUAL2E uses a predictive equation for the saturation (equilibrium) concentration of dissolved oxygen (APHA, 1985).

$$\ln O^* = -139.3441 + 1.575701 \times 10^5 / T - (6.642308 \times 10^7 / T^2) + (1.2438 \times 10^{10} / T^3 - 8.621949 \times 10^{11} / T^4) \quad (6)$$

where,

- O* = equilibrium oxygen concentration at 1 atm , (mg/l)
 T = temperature ($^{\circ}\text{K}$) = ($^{\circ}\text{C} + 273.15$) and $^{\circ}\text{C}$ is within the range 0 - 40 $^{\circ}\text{C}$.

1.4.3 Atmospheric Reaeration Co-efficient

The atmospheric reaeration co-efficient (K_2) is most often expressed as a function of stream depth and velocity. QUAL2E provides eight options for estimating or reading in K_2 values.

- Option 1: Allows to read in K_2 values that have selected by the modeler. This option is useful in modeling unusual situations such as ice cover.
- Option 2: Based on equation given by Churchill, Elmore, and Buckingham (1962). In this option, the model computes the K_2 values for different reaches.
- Option 3: Based on equation proposed by O'connor and Dobbins (1958) . In this option, the model computes the K_2 values for known depth, dispersion coefficient and velocity.
- Option 4: Based on equation proposed by Owens et.al (1964). In this option, the model calculate the K_2 values for known depth and velocity. This option has been found suitable for depths between 0.4 ft to 11 ft. and velocities of 0.1 to 0.5 ft/sec.
- Option 5 : Based on equation proposed by Thackston and Krenkel (1966). In this option, model calculates the K_2 values for different stretches.
- Option 6: Based on equation proposed by Langbien and Durum (1967). For known depth and velocity, the model compute the K_2 values for different reaches.
- Option 7: This option computes the reaeration co-efficient from a power function of flow as shown in the case of velocity and depth. This relationship is to be developed from filed data.
- Option 8: Based on the concept of Tsivoglou and Wallace (1972) where it has been derived that K_2 for areach is proportional to the change in elevation of the water surface and inversely proportional to the flow time through the reach. For given energy slope and known velocity the model compute the K_2 values in this option.

There are no default K_2 values in QUAL2E. The user has to specify any K_2 options as given above.

1.4.4 Carbonaceous BOD

The QUAL2E model assumes a first order reaction to describe deoxygenating of ultimate carbonaceous BOD in the stream. The BOD function as expressed in the model also takes into account additional BOD removal due to sedimentation, scour and flocculation, which do not exert an oxygen demand. Mathematically:

$$\frac{dL}{dt} = -K_1L - K_3L \dots \dots \dots (7)$$

where,

- L = the concentration of ultimate carbonaceous BOD, mg/l
- K_1 = deoxygenating rate co-efficient, temperature dependent, day⁻¹
- K_3 = the rate of loss of carbonaceous BOD due to settling, temperature dependent, day⁻¹

QUAL2E simulates ultimate BOD in the general case; however, the model has the option of 5-day BOD values for input and output. In that case, the model makes the necessary conversions from 5-day to ultimate BOD. The conversion equation is:

$$BOD_5 = BOD_u(1.0 - \exp(-5.K_1)) \dots\dots(8)$$

where,

$$BOD_5 = 5\text{-day BOD, mg/l}$$

$$BOD_u = \text{ultimate BOD, mg/l}$$

$$K_1 = \text{BOD conversion rate coefficient, day}^{-1}$$

1.4.5 Temperature

Temperature is modeled by performing a heat balance on each computational element in the system. The heat balance accounts for temperature inputs and losses from the forcing functions as well as the heat exchanged between the water surface and the atmosphere. The air-water heat balance term include long and short wave radiation, convection, and evaporation using

$$H_n = H_{sn} + H_{an} - H_b - H_c - H_e \dots\dots(9)$$

where

$$H_n = \text{net heat flux passing the air water surface, Btu/ft}^2\text{-day.}$$

$$H_{sn} = \text{net short wave solar radiation after losses from absorption and scattering in the atmosphere and by reflection at the interface BTU/ft}^2\text{-day.}$$

$$H_{an} = \text{net long wave atmosphere radiation after reflection, Btu/ft}^2\text{-day}$$

$$H_b = \text{outgoing long wave back radiation, btu/ft}^2\text{-day.}$$

$$H_c = \text{convective heat flux, Btu/ft}^2\text{-day.}$$

$$H_e = \text{heat loss by evaporation, Btu/ft}^2\text{-day.}$$

To perform the heat balance computation in QUAL2EW, variety of data including the longitude and latitude of the basin, the time of year, evaporation coefficients, and a dust attenuation co-efficient are necessary as inputs. Local climatological information in the form of time of day, wet and dry bulb air temperature, atmospheric pressure, cloud cover and wind velocity are also required.

1.4.6 Temperature dependence of rate coefficients

The temperature values computed in QUAL2E are used to correct the rate co-efficient in the source/sink terms for the other water quality variables. These co-efficient are input at

$$K_T = K_{20}\theta^{(T-20)} \dots\dots\dots(10)$$

20 C and are then corrected to temperature using a Streeter Phelps type formulation.
 where K_t = the value of the coefficient at the local temperature.
 K_{20} = the value of the co-efficient at standard temperature, (20 C)
 θ = an empirical constant for each reaction co-efficient.

1.4.7 Nitrogen cycle

In natural aerobic waters, there is a step wise transformation from organic nitrogen to ammonia, to nitrite, and finally to nitrate. The nitrogen cycle in QUAL2E contains all four of these components. The differential equations governing transformations of nitrogen from one form to another are given below;

(i) Organic Nitrogen

$$\frac{dN_1}{dt} = \alpha_1 \rho A - \beta_2 N_1 - \alpha_4 N_1 \dots\dots\dots(11)$$

where,

- N_1 = concentration of organic nitrogen, mg-N/l.
- β_3 = rate constant for hydrolysis of organic nitrogen to ammonia nitrogen, temperature dependent, day⁻¹.
- α_1 = fraction of algae biomass that is nitrogen, mg-N/mg-A

(ii) Ammonia Nitrogen

$$\frac{dN_1}{dt} = \beta_3 N_1 - \beta_1 N_1 + \frac{C_3}{d} - F_1 \alpha_1 \mu A \dots\dots\dots(12)$$

Where,

$$F_1 = \frac{P_n N_1}{(P_n N_1 + (1 - P_n) N_3)} \dots\dots\dots(13)$$

- N_1 = the concentration of ammonia nitrogen, mg-n/l
- N_3 = the concentration of nitrate nitrogen, mg-N/l

- F_1 = fraction of algae biomass which is nitrogen , mg-N/mg-A.
 P_n = Preference factor for ammonia nitrogen (0 to 1.0).

(iii) Nitrite- Nitrogen

$$\frac{dN_2}{dt} = \beta_1 N_1 - \beta_2 N_2 \dots \dots \dots (14)$$

(iv) Nitrate Nitrogen

$$\frac{dN_3}{dt} = \beta_2 N_2 - (1 - F)\alpha_1 \mu A \dots \dots \dots (15)$$

1.4.8 Phosphorus cycle

QUAL2E only includes dissolved phosphorus to simulate the interactions between organic and dissolved phosphorus. Organic forms of phosphorus are generated by the death of algae, which then convert to the dissolved inorganic state, where it is available to algae for primary production. The differential equations governing transformations of phosphorus from one form to another are given below.

(i) Organic Phosphorus

$$\frac{dP_1}{dt} = \alpha_2 \rho A - \beta_4 P_1 - \hat{c}_5 P_1 \dots \dots \dots (16)$$

where,

- P_1 = concentration of organic phosphorus, mg-p/L
 α_2 = phosphorus content of algae, mg P /mg-A,
 β_4 = organic phosphorus decay rate, temperature dependent , day.
 \hat{c}_5 = organic phosphorus settling rate, temperature dependent, day-1.

(ii) Dissolved Phosphorus

$$\frac{dP_2}{dt} = \beta_4 P_1 + \hat{c}_2 - \alpha_2 \mu A \dots \dots \dots (17)$$

where,

- P_2 = concentration of inorganic or dissolved phosphorus mg -P/l.
 \hat{c}_2 = benthos source rate for dissolved phosphorus, temperature dependent, mg-P/L-day.

1.4.9 Dam Reaeration

QUAL2E has the capability of modelling of oxygen input to the system from reaeration over dams. the following equation described by Butts and Evans (1983) has been used to estimate oxygen input from dam aeration.

$$D_s - D_b = \left(1 - \frac{1}{(1 + 0.116abH(1.0 - 0.034H)(1 + 0.46T))}\right) D_a \dots \dots \dots (18)$$

where,

- Da = oxygen deficit above dam, g/l
- Bb = oxygen deficit below dam, mg/l
- H = height through which water falls
- a = empirical water quality factor
 - = 1.80 in clear water
 - = 1.60 in slightly polluted water
 - = 1.0 in moderately polluted water
 - = 0.65 in grossly polluted water.
- b = empirical dam aeration co-efficient
 - = 0.70 to 0.90 for flat broad crested weir
 - = 1.05 for sharp crested weir with straight slope face
 - = 0.80 for crested weir with vertical face
 - = 0.05 for sluice gates with submerged discharge

The factors, H , a and b are input for each dam.

1.5 Input Data for QUAL2E

QUAL2E accepts hydrological and water quality data through 16 input data cards. PC version of QUAL2E compatible with pC/386 and above has the interface facility for direct accessing of input data on the screen. It is possible, as discussed above to simulate an individual parameter or multiple parameters by mode. Data cards can be prepared according to interest simulation of parameters. Parameters which is are of not interest can bypassed putting the value as “)”, if no value is assigned Under mentioned sections indicate the preparation of data cards as required for the model.

1.5.1 Discretization of River Stretch

The first task that involves to fulfill the requirement of QUAL2E model is the discretization of the river stretch into number of reaches, and to choose the length of computational elements. Length of computational element should be such that total number of computational elements in each reach should not exceed 20. However, the length of computational element could be of any magnitude but should be uniform for all reaches. Smaller the computational element length means requirement of more computer memory but better details

of computation would be obtained, once reaches and the computational elements are discretized, the task left is to identify the functional elements, i.e., the element in which point load, withdrawal, and tributary meet (fig).

1.5.2 Characterization of Hydraulic Parameters and Discharge Coefficients

Hydraulic parameters viz., flow, velocity, depth and Manning's roughness coefficients are important input parameters of the model to compute the oxygen balance in each segment/reach. However, the model does not accept these parameters directly (except the manning roughness coefficient) but accept in the form of coefficient and exponent of velocity, coefficient and exponent of depth which are to be computed from the field observation of velocity, depth, and width of the river at selected locations over the years. Stage-discharge, velocity-discharge, and width -discharge curves developed from at least several consecutive years record would provide the realistic computation.

1.6.3 Flow Balance

Principle of conservation of mass being the basic concept of the model formulation, hydrologic balance in terms of flow in each reach, i.e. flow entered in the reach and out of the reach should be equal. In order to balance the flow in each reach, difference of flow in and out of the reach has been distributed uniformly over the reach as incremental flow into the reach.

1.5 Uncertainty Analysis in QUAL2E

One of the first steps in the chain of risk assessment being the quantification of the errors in predicting water quality, uncertainty analysis has been the subject of much discussion in the ecosystem modeling aspect. Realizing the needs, systematic approach to uncertainty analysis for the general purpose has been incorporated in the QUAL2E which has come as QUAL2E-UNCAS. the objective was to provide some of the tools for incorporating uncertainty analysis as an integral part of the water quality modelling process. Three uncertainty analysis techniques has been employed in QUAL2E-UNCAS-sensitivity analysis , first order analysis, and monte-carlo simulation. Monte carlo simulation has the advantage of output frequency distributions, but it carries a high computational burden while first order propagation provides a direct estimate of model sensitivity, but that variability is usually more indicative of the variance of model components than of the dynamics of the model structure. Therefore, QUAL2E is one of the most efficient water quality model with broad application facilities for surface water quality modeling

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