

STATE OF ART REPORT

Scientific Contribution
No. : INCOH/SAR-14/97

SURFACE WATER QUALITY MODELLING - STATE OF ART IN INDIA

Vijay Joshi

INDIAN NATIONAL COMMITTEE ON HYDROLOGY
(Committee Constituted by Ministry of Water Resources, Govt. of India)



INCOH SECRETARIAT
NATIONAL INSTITUTE OF HYDROLOGY
ROORKEE - 247 667, INDIA

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PREAMBLE

It has been estimated that the total world population will be around 6.5 billion by the year 2000, with the most rapid growth in the developing countries. By that time, the countries within the humid tropics and the other warm humid regions will represent almost one-third of the total world population. This proportion will continue to rise in the 21st century. The developing and under-developed countries thus quite clearly are the regions facing potentially serious water problems. Hence, it is urgent to question as to whether the fields of hydrology and water resources management have the appropriate methods in place to meet the rising demands that will be made on the water resources. Hence it becomes very important and expeditious to review and update the state-of-art in different facets of hydrology and component process. This calls for compiling and reporting present day technology in assessment of water resources and determining the quality of these water resources.

The Indian National Committee on Hydrology is the apex body on hydrology constituted by the Government of India with the responsibility of coordinating the various activities concerning hydrology in the country. The committee is also effectively participating in the activities of UNESCO and is the National Committee for International Hydrology Programme (IHP) of UNESCO. In pursuance of its objective of preparing and periodically updating the state-of-art in hydrology in the world in general and India in particular, the committee invites experts in the country to prepare these reports on important areas of hydrology.

Realising the important role of water quality modelling in the overall planning of water resources, the committee decided to invite an expert for preparing the status of water quality modelling in India. Water quality modelling is not new; it is as old as about 75 years. The first water quality modelling studies were conducted on Ohio river in 1925 for two most conventional pollutants namely DO and BOD. Thereafter, lot of works have been carried out by different experts. In India also, though limited, yet extensive capabilities have been developed by various institutes and experts. Basically, the modelling of surface water quality has two fold results- a) better understanding of the mechanism and interactions that give rise to various water quality behaviours, such understanding needs to be sharpened by the formulation and testing of hypothesis of the cause-effect relationship between residual inputs and resulting water quality and b) modelling efforts provide a more rational basis for making water quality control decisions to include a defensible, credible, predictive framework within the larger framework of cost-benefit analysis. With the objective of re-

viewing capabilities in water quality modelling and realizing the urgent need to do so, the present report has been written.

The Indian National Committee on Hydrology with the assistance of its erstwhile Panel on Water Quality, Erosion and Sedimentation has identified this important topic for preparation of this state-of-art report and the report has been prepared by Dr. Vijay Joshi, Senior Scientist, NEERI, Bombay Zonal Laboratory. The guidance, assistance and review provided by the Panel are worth mentioning. The report has been compiled and finalised by Dr. K.K.S. Bhatia, Member-Secretary and Sri R. Mehrotra, Scientist-in-charge, Indian National Committee on Hydrology.

It is hoped that this state-of-art report would serve as a useful reference material to practising engineers, researchers, field engineers, planners and implementation authorities, who are involved in correct estimation and optimal utilization of the water resources of the country.



(S.M. Seth)

Executive Member, INCOH
& Director, NIH

Roorkee

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INTRODUCTION

A large number of pollutants find their way into the surface water bodies due to their increased use for waste disposal. Subsequent to their disposal, the pollutants undergo a set of complex transformations as they get transported in the water body. The result of these transformations, through the process of self assimilation of the water body, is a net decrease in the level of pollutants with time. An overuse of these bodies, however, could result into significant deterioration of the water quality.

For instance, significant oxygen depletion can occur at downstream reaches of a slow moving river receiving large discharges of biodegradable organics. Similarly, sustained disposal of inadequately treated industrial waste in lake could built up the nutrient levels giving rise to an algal bloom under adverse meteorological conditions. To protect the water bodies for their abstractive and instream uses, it is necessary to control their assimilative use by means of effluent and/or surface water quality standards.

Rational decisions on the intensity of such control measures warrant reasonable a priori estimates of the impact of wastewater discharges on the receiving waters. Similar considerations are necessary for optimal siting of monitoring locations and frequency for surveillance and obtaining spatial and temporal trend of water quality in a water body.

Water quality models attempt to provide such estimates by describing the relevant transformation processes by constructing an approximate mathematical equivalent of the actual system. These models provide efficient tools for the design of water quality management or monitoring programmes. For instance, relative merits of different wastewater management schemes could be evaluated by assessing their impacts on the receiving water bodies using the water quality models for the water body.

SCOPE OF THE REPORT

The process of development of a water quality model for a water body essentially comprises four major steps in the form of

- I. Collection of deductive information and data
- II. Selection of suitable mathematical structure
- III. Model calibration
- IV. Model verification and validation.

All of these four steps are intimately related and the procedure of model development invariably involves repetition of some or all of these in systematic manner. This report in the following sections provides a general introduction to these areas. The material presented herein is confined to the rivers and estuaries and does not include lakes and reservoirs. The developments till late eighties have been covered for India.

COLLECTION OF DEDUCTIVE INFORMATION AND DATA

The first step in water quality model development concerns with obtaining as much information as possible about the system by means of theoretical investigations, in situ measurements and laboratory experiments. The objective of this study normally is to filter out those transformation processes from the model structure which do not appear to have an appreciable affect on the water quality parameters of interest. The end use of the model also plays an important role in such eliminations. For instance, in a rapidly flowing river receiving untreated wastewaters the affect of decay of nitrogenous BOD can not be significant on the river DO system for a considerable longitudinal distance. If the end use of the water quality model is design of monitoring network for surveillance near large towns receiving multiple wastewater discharges, decay component for nitrogenous BOD can be eliminated from the model structure.

Similarly, information on a river stretch on nutrient and algal concentrations could be used to eliminate or incorporate the mechanism of photosynthesis while modelling dissolved oxygen. Development of relationships among Chlorophyll-a and algae biomass for specific species of Algae, rate of oxygen production with sunlight intensity etc. are the laboratory experiments which can yield valuable information on initial estimates of model parameters related to photosynthesis.

Information on channed characteristic and river flows is also essential for setting up a suitable mathematical model and identification of critical conditions for modelling. Information on river velocities and bottom deposits downstream a wastewater discharge could lead to the decision on inclusion of BOD removal by settling or its addition by scouring or providing for a distributed DO sink in the river water quality model.

Data collection for the development of a matematical model for a riverine or estuarine section is an elaborate and specialized activity. The routine water quality and flow observations on these systems generally do not provide adequate information on important aspects necessary for even simple mathematical models, and therefore are not adequate for model development. Such data bases, however, have potential to be used as important information source for the identification of dominant transformation processes in the system and data gaps for further strenghtening of the data collection programmes.

Through the sustained efforts of Central Pollution Control Board (CPCB), State Pollution Control Boards, Central Water Commission and project undertaken by Ganga Project Directorate (GPD), sufficient information is now available on Ganga and Yamuna rivers to identify the critical river reaches, water quality parameters and critical periods for modelling (1,2,3). CPCB has also carried out a water quality assessment and wastewater inventory programme on River Chambal downstream of Kota. Under the Global Environmental Monitoring Scheme regular information is also being collected to provide a general picture of the state of water quality (4). Under the Assessment & Development Study of River Basin Series, CPCB regularly compiles and publishes recent information on river water quality in Indian rivers. These data, though provide very useful insight into the water quality status in these rivers, are not adequate for meaningful modelling exercise with the exception of perhaps the data on River Yamuna downstream of Delhi.

Q

STRUCTURE IDENTIFICATION

The step of selection of an appropriate model structure on the basis of theoretical or empirical considerations is known as structure identification. There are generally two approaches for structure identification. The first of these approaches, which is very popular in the field of water quality modelling, represents the mathematical structure of the model through cause - effect type relationships. This approach involves the conceptual subdivision of the water quality system into smaller, individual components whose (conceptual) behaviour can usually be approximated by laboratory-scale replicas. It is assumed that the submodels describing these components can be verified and the model for the field system can be assembled by certain causative linkages of the submodel(5). Such models are known as causal models.

The second approach for development of water quality models uses the in situ data collected on the system for identifying the model structure by means of statistical techniques such as time series analysis, correlation analysis and Group Method of Data Handling (GMDH) for obtaining the mathematical representation of the model (6). The statistical techniques are generally data intensive and are of limited use for modelling those modes of system behaviour which are not captured in the past data. For instance, a statistical model developed through the data collected on a polluted river stretch would be of limited use for generating scenarios for evaluating a set of wastewater abatement measures which shall significantly alter (improve) the ambient (polluted) water quality in the river.

The casual models, however, can be adapted to changed water quality conditions with adjustments in model variables based on theoretical and empirical reasoning. In Indian context, most of the application in riverine and estuarine water quality modelling are that of causal models.

Mathematical Formulation

The important processes which affect a water quality constituent in the rivers and estuaries are advection, dispersion and decay or growth due to chemical biochemical reactions. Since the depth and width of these water bodies are generally much less than 0 the longitudinal distance over which the water quality variations are of interest, in most

cases vertical and lateral homogeneity is assumed while modelling river water quality. Under these assumptions one-dimensional advective-diffusion equation for reactive substance forms the basis for river water quality models and can be written as (7),

$$\frac{\partial s}{\partial t} = - \frac{1}{A_x} \frac{\partial}{\partial x} (SQ) + \frac{1}{A_x} \frac{\partial}{\partial x} (EA_x \frac{\partial s}{\partial x}) \pm Ks \pm S_d \quad \dots(1)$$

Where,

- s(x,t) : Concentration of water quality
- Q : River flow
- A_x : Cross-section area at locations x
- E : Longitudinal dispersion coefficient at location x
- K : Decay or growth rate coefficient assuming a first order reaction.
- S_d : Amount of materials added to (or withdrawn from the stream per unit time) due to distributed source or sink

In Eq. 1 the terms on the right hand side respectively represent the processes of advection, longitudinal dispersion, decay or growth due to chemical or biochemical reaction and a source or sink that is already distributed in the river due to some previous phenomenon.

Use of numerical methods is necessary to obtain the solution of such equations. Modelling of most water quality constituents also entails solution of a set of coupled equations of the form shown in Eq. 1. Qual-II developed by US Environmental Protection Agency (EPA), is generally considered as most elaborate causal water quality model suitable for quasi-dynamic simulation of 1-dimensional rivers and estuaries neglecting the inter tidal variations (8). The set of coupled differential equations used in the model along with the range of values for model coefficients and causative links between the submodels for different water quality parameters are given in Annexure-I. The model though considers the temporal variations of water quality parameters due to diurnal variations in sunlight etc., it does not support variations in river and wastewater flow with time. The model has been extensively used by the National Institute of Hydrology, Roorkee including the latest versions. The model has been successfully used for river Kali in U.P. (9). Attempts are also being made to use on river Krishna (10). The model is available including the source code for the computer programme with National Environmental Engineering Research Institute (NEERI) and has been applied for water quality simulation in environmental assessment studies for a large variety of cases in India.

Temporal/Overall Model for Catchment (TOMCAT) is another versatile model for 1-dimensional modelling of rivers available in India with GPD. TOMCAT developed by Thames Water Authority, UK, addresses the water quality simulation in much simpler form compared to QUAL-IIIE, using steady state form of EQ.1 without longitudinal dispersion and for a restricted choice of water quality parameters and transformation processes (11). The model, however, take into account the diurnal variations in wastewater and river flows with the help of Monte Carlo Simulation. Relevant details of mathematical structure and other important features of the model are given in Annexure -II.

Other computer models readily available in India which address the problem of river water quality modelling in comparable details are stochastic water quality model for river Seine which can readily be adapted to other river systems (12) and STREAM I developed by IIT Bombay (13). For steady state and predominantly advective flow the governing equations for 1-dimensional river simulation take very simple form of first order linear differential equations which are easily intergrable and may be in use by many research workers. The analytical solution of these equations for a large number of subsystems are provided by Willis et, al (14).

For a number of wide river in which lateral variation of water quality are also important, the assumption of 1-dimensional consideration is not applicable. For modelling of such rivers, specially for the stretches downstream of the major towns and industrial clusters, it is necessary to take recourse to 2-dimensional consideration. Depth intergrated 2-dimensional advective-diffusion equation provide the mathematical framework for modelling of such systems which in curvilinear co-ordinate system is expressed as (15).

$$m_x m_z \frac{\partial(hc)}{\partial t} + \frac{\partial}{\partial x} (m_z huc) + \frac{\partial}{\partial z} (m_x hvc) \frac{\partial s}{\partial x} \left(\frac{m_z}{m_x} h e_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial z} \left(\frac{m_x}{m_z} h e_x \frac{\partial c}{\partial z} \right) \dots(2)$$

where t = time; x,z = longitudinal and transverse distance in orthogonal curvilinear system ; u,v = depth-averaged velocity components in the x,z, direction ; h = local flow depth; c = depth-averaged concentration, e_x, e_z = turbulent mixing or dispersion coefficients in the x,y direction ; and m_x, m_z = metric coefficients for the coordinate system.

Computer codes for solution of above equations after a few simplifications by analytical techniques as well as numerical methods are available at NEERI and IIT Bombay.

Models incorporating analytical solution are also available at SJ College of Engineering Mysore. These codes in their present form restrict the scope of water quality simulations to DO-BOD interaction in the river arising out of the processes of decay of carbonaceous organic matter and reaeration. The computer codes, however, can readily be adopted to include other relevant transformation processes. Further details of these formulations are provided in Joshi et. al. (16), Modak et. al. (13) and Gowda (17, 18). Bhatia (19), Ghosh (20) have provided comprehensive review of water quality models.

For detailed water quality simulation for estuaries, often, a truly dynamic modelling framework in two dimensions is necessary. The modelling considerations entail solution of depth integrated continuity and momentum conservation equations for shallow water bodies using finite difference schemes. the solution of these equation provide the hydrodynamic response of the model for changes in current and water depths arising out of tidal forcing. The mass-balance equations for the pollutants' concentration are then solved to obtain the concentration profiles. The codes available in India for the solution of such equations include the model TIDAL available at Centre For Mathematical Modelling and Computer Simulation, NAL, Banagalore (21), WASP3 at NEERI (22) and unpublished inhouse developments at Centre for Water and Power Research Station (CWPRS), Pune and IIT Dehi. A pictorial presentation of the processes incorporated in model TIDAL are provided in Annexure-III. WASP3 also incorporates similar processes. TIDAL, however, is more user friendly and provides the facility for graphical presentation of the model results.

The available information on the river or estuarine system plays a important role in the step of structure identification. For riverine or estuarine water quality systems where numerous complex reactions affect the concentration of water quality constituents, the step of model identification is not amenable to a simple analysis. Due to the difficulties in interpreting the results of large models (with many submodels and processes) and associated ambiguity in model calibration, it is advisable that a model building procedure should be initiated with a simple model structure catering to only the dominant transformation processes observed in the system. Addition components should be added to this structure only when the step of model calibration provides unrealistic or inexplicable values of model parameters for these processes.

MODEL CALIBRATION

The step of model calibration (also known as parameter estimation) essentially involves the tuning of the model through the coefficients occurring in the model structure such that the model output provides a reasonable match with the observations obtained on relevant water quality constituents. Following two procedures are generally used for model calibration,

- (i) Method of trial and error
- (ii) Method based on an estimation criterion

In trial and error method the model response is obtained for certain set of model parameters and is manually compared with the observed values of water quality constituents obtained during the field survey. If the model output do not match reasonably well with the observations, the parameter values are changed to improve the fit of model response with the observations. The success of this procedure greatly depends upon the extent of complexity of the system, reliability and depth of available data and the experience of the modeller.

Alternatively, an estimation criterion such as Normalised Root Mean Square Error (NRMSE) or Root Mean Square Error (RMSE) can be used to provide the estimate of difference between model response and observation and can be minimized by a constrained non-linear optimization technique (23).

Concurrent observations on river flows, major wastewater discharge and water quality constituents at a number of locations are necessary to achieve a reasonable success in the modelling exercise. For deciding the time of sample collection at different river locations, it is also necessary to conduct time of travel studies using chemical or radioactive tracers. Since for developing a 1-dimensional model for a river stretch, water quality observations over a distance travelled by the river in two to three days time are required, considerable monitoring effort is needed for data collection.

In view of above, special data collection programmes of about 15 days duration for each stretch on a river are necessary for model calibration. Only two such efforts, first on river Ganga at Varanasi during June 1989 by NEERI and second on River Hoogly in April, 1991 by Thames Water and CPCB team have been made in India. Due to insufficient

equipment and laboratory support, NEERI's effort of 1989 which was directed towards calibration of 2-dimensional water quality model, did not provide adequate data for model calibration. Details and achievements of the effort on river Hooghly can be obtained from GPD. NEERI has also conducted a data collection exercise on Malad Creek near Bombay for hydrodynamic and water quality model calibration. NIH has taken up extensive data generation programme for using QUAL-III for river Kali (U.P.).

In the absence of water quality data, specially collected for water quality modelling, certain efforts have been made by using available data for performing preliminary modelling exercises on the rivers specially on Ganga, Krishna and Yamuna. The first major attempt on river Ganga was done by the author in 1987 by using water quality data collected by CPCB and flow data collected by CWC. In the course of this work DO-BOD interaction over the complete riverine portion of river Ganga upstream Farakka were modelled using the model TOMCAT.

Estimate of reaeration coefficient were obtained through the use of COVAR diagram (24). The estimates of carbonaceous BOD decay coefficients were obtained through manual calibration. Later through a sponsored project by GPD, certain modelling efforts on river Ganga were carried out at IIT Bombay (1988-90). CPCB has also carried out certain modelling exercise on river Yamuna downstream of Delhi. Earlier Bhatia has conducted DO-BOD modelling using DOSAG-1 model for the river Hindon (25). The details of these works can be obtained through the respective organizations.

For successful calibration it is necessary that calibrated model parameters fall within a physically meaningful range and their variations over different reaches can be explained based on the changes in river hydraulic characteristics, confluence of major tributary or wastewater discharge etc. If the estimated values of model parameters exhibit behaviour which is not in harmony with their physical attributes, it may reflect inadequacy in either

- (i) observations
- (ii) structure identification, or
- (iii) both

and necessitate repetition of these steps. However, it is advisable to attempt to resolve these oddities of model parameters by making suitable alteration in model structure before collecting the observations a fresh.

MODEL VERIFICATION AND VALIDATION

The step of model verification in model building process provides a means for quick evaluation of the success of model identification and calibration before the model is put to more rigorous field tests. In this step, a portion of data not used for model calibration before the model is put to more rigorous field tests. In this step, a portion of data not used for model calibration is used to check the effectiveness of model predictions. If model predictions are found to tally with the actual observations satisfactorily, the model is said to be verified, otherwise the previous steps of model building procedure are repeated yet another time. As there has been a little effort in the area of calibration of water quality models in India there are no reported studies which address the problem of model verifications in the right earnest.

Model validation can be regarded as a means of evaluating model's ability to predict correct future behaviour of the system under substantially changed conditions. Evidently model validation requires collection of field data under different conditions of system inputs and river flow conditions than those for which model has been calibrated. In the absence of such information on the system, model validation is carried out by changing various model inputs over a wide range and studying model outputs for inexplicable anomalies in system behaviour.

CONCLUSIONS

Pollutants, once discharged into a river, undergo a variety of complex interrelated biochemical and physical transformations. When the prediction of their impact on river water quality along the longitudinal direction is of interest, 1-dimensional advective diffusion equation with growth/decay and source/sink terms and appropriate initial and boundary conditions provides the necessary basis for mathematical simulation of water quality. For wide rivers, however, it is necessary to formulate the problem in 2-dimensions. Solution of depth averaged continuity, momentum conservation and mass transport equations is necessary to consider inter-tidal variation in most estuaries.

Due to the complex nature of water quality system, success in satisfactory simulation is normally hard to achieve. A systematic field survey for collection of data on in situ river water quality, wastewater discharge characteristics and river hydrological parameters are necessary prerequisite for model development. It is also obligatory on the part of the modeller that the steps of model identification, model calibration and model verification and validation be objectively followed before the model is put to use in practice.

In Indian context, adequate software support is available to undertake detailed modelling studies of riverine and estuarine water quality systems. There is, however, a need to create an organizational infrastructure which can undertake intensive coordinated monitoring efforts necessary to generate data for model calibration and verification.

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Annexure - I

MATHEMATICAL EQUATIONS AND SUBMODEL LINKAGES OF MODEL QUAL-IIe

Conservative mineral (C)
$$\frac{\partial c}{\partial t} = \frac{\partial(A_x E \frac{\partial c}{\partial x})}{A_x \partial x} - \frac{\partial(A_x UC)}{A_x \partial x} + \frac{S_c}{A_x \Delta X}$$

Algae (A)
$$\frac{\partial A}{\partial t} = \frac{\partial(A_x E \frac{\partial A}{\partial x})}{A_x \partial x} - \frac{\partial(A_x UA)}{A_x \partial x} + \frac{S_A}{A_x \Delta X} + (\mu_A - \rho - \frac{\sigma_1}{D_0}) A$$

Ammonia nitrogen (NH₃)

$$\frac{\partial NH_3}{\partial t} = \frac{\partial(A_x E \frac{\partial NH_3}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \partial UNH_3)}{A_x \partial x} + \frac{S_{NH_3}}{A_x \Delta X} + (\alpha_1 \rho^A - \beta_1 NH_3 + \frac{\sigma_3}{A_x})$$

Nitrite nitrogen (NO₂)

$$\frac{\partial NO_2}{\partial t} = \frac{\partial(A_x E \frac{\partial NO_2}{\partial x})}{A_x \partial x} - \frac{\partial(A_x UNO_2)}{A_x \partial x} + \frac{S_{NO_2}}{A_x \Delta X} + (\beta_1 NH_3 - \beta_2 NO_2)$$

Nitrate nitrogen (NO₃)

$$\frac{\partial NO_3}{\partial t} = \frac{\partial(A_x E \frac{\partial NO_3}{\partial x})}{A_x \partial x} - \frac{\partial(A_x UNO_3)}{A_x \partial x} + \frac{S_{NO_3}}{A_x \Delta X} + (\beta_2 NO_2 - \alpha_1 \mu_A A)$$

Phosphate phosphorus (P)

$$\frac{\partial P}{\partial t} = \frac{\partial(A_x E \frac{\partial P}{\partial x})}{A_x \partial x} - \frac{\partial(A_x UP)}{A_x \partial x} + \frac{S_P}{A_x \Delta X} + [\alpha_2 (\rho - \mu_A) A - \frac{\sigma_2}{A_x}]$$

Contd...

Biochemical oxygen demand
(BOD')

$$\frac{\partial \text{BOD}^c}{\partial t} = \frac{\partial(A_x E \frac{\partial \text{BOD}^c}{\partial x})}{A_x \partial_x} - \frac{\partial(A_x \text{UBOD}^c)}{A_x \partial_x} + \frac{S_{\text{BOD}^c}}{A_x \Delta X} - (K^c + K_3) \text{BOD}^c$$

Benthic oxygen demand (BOD^b)

$$\frac{\partial \text{BOD}^b}{\partial t} = \frac{(A_x E \frac{\partial \text{BOD}^b}{\partial x})}{A_x \partial_x} - \frac{\partial(A_x \text{UBOD}^b)}{A_x \partial_x} + \frac{K_b}{A_x}$$

Dissolved oxygen (DO)

$$\frac{\partial \text{DO}}{\partial t} = \frac{\partial(A_x E \frac{\partial \text{DO}}{\partial x})}{A_x \partial_x} - \frac{\partial(A_x \text{UDO})}{A_x \partial_x} + \frac{S_{\text{DO}}}{A_x \Delta X}$$

$$+ [K_\alpha (\text{DO}_x^{\text{SAT}} - \text{DO}) + (\alpha_3 \mu_A - \alpha_A \rho) A - K^c \text{BOD}^c - \frac{K_b}{A_x} - \alpha_5 \beta_1 \text{NH}_3 - \alpha_6 \beta_2 \text{NO}_2]$$

Coliform (F)

$$\frac{\partial F}{\partial t} = \frac{\partial(A_x E \frac{\partial F}{\partial x})}{A_x \partial_x} - \frac{\partial(A_x \text{UF})}{A_x \partial_x} + \frac{S_F}{A_x \Delta X} - K_d F$$

Radioactive material (R)

$$\frac{\partial R}{\partial t} = \frac{\partial(A_x E \frac{\partial R}{\partial x})}{A_x \partial_x} - \frac{\partial(A_x \text{UR})}{A_x \partial_x} + \frac{S_R}{A_x \Delta X} - \gamma_r R - \gamma_\alpha R$$

INPUT PARAMETERS FOR QUAL-IIe

Symbol in equaiton Description	Uints	Range of values	Reliability
α_0 Ratio of chlorophyll a	$\frac{\mu\text{gChl a}}{\text{mg A}}$	50-100	Fair
α_1 Fraction of algae biomass which is NO_3	$\frac{\text{mg N}}{\text{mg A}}$	0.08_0.09	Good
α_2 Fraction of algae biomass which is P	$\frac{\text{mg P}}{\text{mg A}}$	0.012_0.015	Good
α_3 O_2 Production per unit of algae growth	$\frac{\text{mg O}}{\text{mg A}}$	1.4_1.8	Good
α_4 O_2 Uptake per unit of algae respired	$\frac{\text{mg O}}{\text{mg A}}$	1.6_2.3	Fair
α_5 O_2 Uptake per unit of NH_3 oxidation	$\frac{\text{mg O}}{\text{mg N}}$	3.0_4.0	Good
α_6 O_2 Uptake per unit of NH_2 oxidation	$\frac{\text{mg O}}{\text{mg N}}$	1.0_1.14	Good
μ^{max} Maximum specifice growth rate of algae	$\frac{1}{\text{day}}$	1.0_3.0	Good
ρ Algae respiration rate	$\frac{1}{\text{day}}$	0.05_0.5	Fair
β_1 Rate constant for biological oxidation of $\text{NH}_3 \rightarrow \text{NO}_2$	$\frac{1}{\text{day}}$	0.1_0.5	Fair
β_2 Rate constant for biological oxidation of $\text{NH}_2 \rightarrow \text{NO}_3$	$\frac{1}{\text{day}}$	0.5_2.0	Fair

Contd...

Symbol in equation Description	Units	Range of values	Reliability
σ_1 Local settling rate for algae	$\frac{\text{ft}}{\text{day}}$	0.5_6.0	Fair
σ_2 Benthos source rate for phosphorus	$\frac{\text{mg P}}{\text{day-ft}}$	Highly Variable	Poor
σ_3 Benthos source rate for NH_3	$\frac{\text{mg N}}{\text{day-ft}}$	Highly Variable	Poor
K^c Carbonaceous BOD decay rate	$\frac{1}{\text{day}}$	0.1_2.0	Poor
K_a Reaeration rate	$\frac{1}{\text{day}}$	0.0_100	Good
K_3 Carbonaceous BOD sink rate	$\frac{1}{\text{day}}$	Highly Variable	Poor
K_b Benthos source rate for BOD	$\frac{\text{mg}}{\text{day - ft}}$	Highly Variable	Poor
Y_y Radionuclide decay rate	$\frac{1}{\text{day}}$	Highly Variable	Poor
K_d Coliform die-off rate	$\frac{1}{\text{day}}$	0.5_4.0	Fair
Y_d Radionuclide absorption rate	$\frac{1}{\text{day}}$		Poor
K_{NO_3} Nitrate-nitrogen half-sat Constant for algae growth	$\frac{\text{mg}}{1}$	0.2_0.4	Fair to good
K_p Phosphorus half-saturation Constant for algae growth	$\frac{\text{mg}}{1}$	0.03_0.05	Fair to good
K_t Light half-saturation constant for algae growth	$\frac{\text{Langley}}{\text{day}}$	260	Good

INPUT PARAMETERS FOR QUAL-IIe

ANNEXURE II

Mathematical Structure and Model TOMCAT

The river water quality model TOMCAT simulates the processes of thermal transfer, natural purification comprising carbonaceous oxidation, oxidation of ammonical nitrogen and oxygen balance considering these processes as sink and reaeration as the source for Dissolved Oxygen.

The basic differential equations used in the model as the following

$$\text{Thermal transfer } \frac{dT}{dt} = -k_T (T_t - T_{\text{air}})$$

where

- T_t : River temperature
- T_{air} : Air temperature
- K_t : Rate constant for thermal transfer

Carbonaceous Oxidation

$$\frac{dB}{dt} = -k_B (B_t - B_{\text{min}})$$

where

- B_t : BOD at time t
- B_{min} : Background BOD_u
- K_B : BOD decay coefficient

Nitrification

$$\frac{dN}{dt} = -K_N (N_t - N_{\text{min}})$$

where

- N_t : Ammonical Nitrogen at time t
- N_{min} : Background Ammonical Nitrogen
- K_n : Coefficient for Ammonical Nitrogen

Oxygen Balance

$$\frac{dC}{dt} = K_R (C_{sat} - C_t) - \frac{dB}{dt} - E \frac{dN}{dt}$$

Where

- K_R : Overall absorption coefficient
 C_t : Dissolved oxygen concentration at time t
 C_{sat} : Dissolved oxygen saturation concentration
 E : Equivalent oxygen demand of a ammonical nitrogen, assume to be 4.57

The model TOMCAT makes use of Monte Carlo simulation technique to solve the above equations for different sets of initial conditions and forcing functions. The model thus can simulate the effect of diurnal variation of wastewater loads on river quality.

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