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AN INTEGRATED OPTIMIZATION MODEL FOR RIVER WATER QUALITY TO ESTIMATE WASTEWATER REMOVAL

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ABSTRACT

River water quality is affected by both point and diffuse sources of pollution. Point sources of pollution include domestic or industrial discharges via pipe connections to the river system, whereas diffuse sources of pollution include runoff from the agricultural land and mining sites. The dynamic integrated modelling of basic water quality and organic contaminant fate and effect in rivers are explored. A basic river water quality model and organic contaminant submodel which using mathematical model then were developed and linked in order to estimate the wastewater removal efficiencies for discharge site.

Keywords: *Water Quality, Waste Water Discharge, Modelling*

INTRODUCTION

Our environment now needs to be protected from every sources of pollution, because humans' survival depends on the sustainable use of natural environment. Rivers as the essential part of environment is also very important in our daily life. Many different pollutants, including conventional pollutants (organic matter and inorganic nutrients) and hazardous substances (organic contaminants and heavy metals) threaten the quality of river nowadays. Although we know that the river water quality can be influenced by natural phenomena such as geology and climate, the main sources of pollution are related to anthropogenic activities such as mining, agriculture, forestry, cattle farming and urbanization (Deksissa [3]). Finally, water quality of river is affected by whole factors including climate, geology, and diffuse sources of pollution. The main sources of pollution themselves are from domestic or industrial discharges via pipe connections to the river system, whereas diffuse sources of pollution include runoff from the agricultural land and mining sites. All of that have resulted in two important problems of water quality in surface waters, they are: eutrophication (nutrient enrichment) and contamination by hazardous organic compounds.

Basically, models of water quality require a relatively large number of parameters to define the functional relationships, and they are commonly defined by fitting the model to observed data, since prior information on parameter values is limited. Those models can be

used to simulate conditions in or near the range of the calibrated or verified conditions. In this case, the estimation of parameters, which is still practiced by heuristic approaches (i.e. manually), presented as the point where the attention needs to be focused.

Rauch et al. [15], stated the art in river summarized modelling of water quality also addressed some issues related to the practical use of river quality models. After make comparison of 10 important software products, they indicated that only two of them which offered limited parameter estimation capability. Gujer et al. [4] also noted that practitioners often resorted to manual trial-and-error curve fitting for calibration. The software product which accepted for river water quality modeling worldwide is U.S. EPA's QUAL2E (Brown and Barnwell, [2, 16]). Actually, this software does not appropriate with the issue of parameter estimation that should address a number of practical problems. Most of practical applications of water quality models, manually chosen the parameter values rather than apply the automated numerical techniques, or heuristic approaches are resorted to [3]. In fact, the automated methods are associated with some difficulties depending on the model's structure, optimization method, number of variables and parameters, type of measurements and so on, something that very needed for simplicity. As result, there is no any automated estimation of parameters for models of river water quality have been reported yet.

Sincock et al. [17] also reported a detail study about how identification of model parameters involved. The result showed that the data were considered relatively scarce, and although temperature was predicted accurately; nitrate, BOD₅ and DO predictions were less so. Based on the fact that the segment of river between sampling stations was assumed to be a completely stirred tank reactor (CSTR), this modelling was created. This particular work was later extended to the series called the CSTR approach [3].

The challenge is appeared to use mathematical modelling such that it can be a support tool to evaluate the water quality remediation options. Most of modelling are expensive and require substantial investments in reliable data, development of scientific capacity and also relatively sophisticated management culture that are often not found in developing countries. But, new developments in water quality police and strategies towards integrated river basin approach require a mathematical model as a tool in water quality management (e.g. [5, 12]). Because both of those monitoring and modelling provide important information for water quality regulator, water quality modelling becomes increasingly important due to its cost-effectiveness and unique predictive. To achieve water quality objectives, various scenario analyses and evaluation of alternative management operation can be used well. Meanwhile, mathematical models describe the complex relationships between waste load from different sources (point or non-point) and the resulting water quality responses.

Several types of basic river water quality models which mainly deal with nutrient and oxygen balance well explained in literature. (Streeter and Phelps, [11]) explained the increasing of the complexity and number of state variables of oxygen sag' model to the extended models such as *QUAL1* (Orlob, [10]), *QUAL2* (Water Resource Engineering, 1973) *QUAL2E* (Brown and Barnwell, [2,16]), *MIKE11* (DHI, 1992), *DUFLOW-EUTROF1* (Alderink *et al.*, [1]) and *ISIS* (Wallingford, [13]). However, none of these models use microbial biomass as state variables despite the fact that microbial biomass determines the rates of biotransformation processes. The Biological Oxygen Demand (BOD) only represent a part of the biologically degradable matter. It means, the mass balance for carbonaceous organic matter depends on it. But, it is really difficult to use BOD for the calculation of mass balances (Henze, [6]). They do not include the particulate organic matter such that the BOD-values are therefore not suitable and hence cannot divide the different organic carbon fractions.

The river water quality task group proposed the River Water Quality Model No. 1 (RWQM1) (Reichert *et al.*, [10]),. The model which is based on Chemical Oxygen Demand (COD) as a measure of carbonaceous organic matter is developed for consistency not only in mass balance but also in elemental balance, similar to the Activated Sludge Models, ASM-1 (Henze *et al.*, [6]), ASM-2 (Henze *et al.*, [8]) and ASM-3 (Gujer *et al.*, [6]). In fact, it is compatible with the activated sludge models, and thus suitable for integrated water quality modelling of urban waste water of rivers (Meirlaen *et al.*, [9]). In RWQM1, COD values are divided into different organic fractions assuming constant elemental composition of compounds and organisms in the system. Then the mass fraction of elements (C, H, O, N and P) is used as model parameters. And the stoichiometric coefficients of conversion processes are formulated as a function of these parameters. Monod-type limitation factors are also used to formulate the biochemical processes. However, RWQM1 is considered too comprehensive and complex to be applied directly in many situations where there are limited available data, including developing countries for instance. This model consists of 24 variables, 36 kinetic parameters, 6 equilibrium parameters, 13 stoichiometric parameters, 36 mass fractions, and as such it requires a large input data set. In addition, the number of state variables and parameters becomes considerably larger when the benthic sediment is also included. It is also difficult to find reliable and sufficient data to calibrate these parameters. Based on the poor data, it needs to focus on a simple river water quality model that respects both mass and elemental balances and is still compatible with the activated sludge models.

MODEL FORMULATION

A simple model was developed based on the simple mass balance in order to control

further deterioration of river water quality which caused by high levels of upstream water abstraction and by contributions of polluted inflows in the downstream reaches of the river.

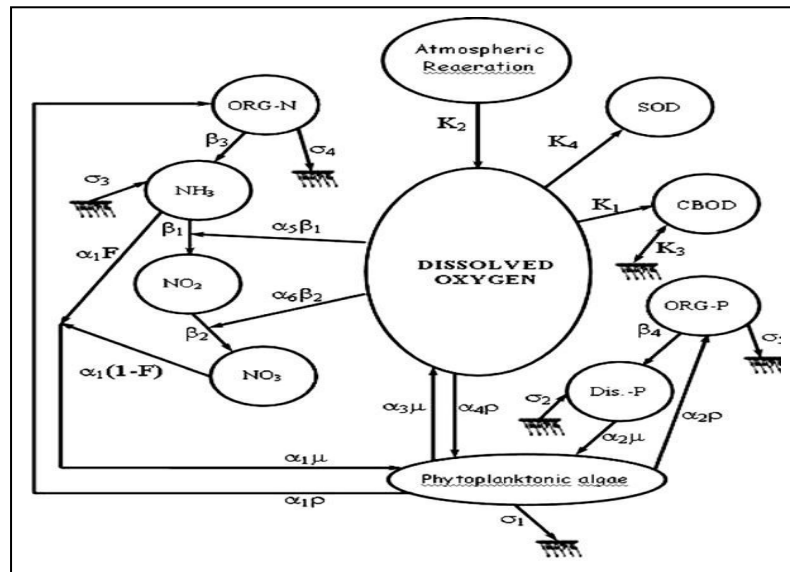


Figure 1. Dissolved oxygen balance and effecting parameters in QUAL2E.

Nowadays, irrigation, industry and domestic water supply is abstracted from the main river or its tributaries. Most of this water will be lost through evaporation and just very little may return to the river. It means an increase of TDS concentrations in the downstream reaches of the river can be happened because of the high rates of water withdrawal at the upstream point or from tributaries in the upper reaches. The fact that the volume of water reaching the downstream sections of the river is too low to dilute the inflows from polluted side streams and /or effluent discharges, so a relatively simple dynamic water quality model consisting of completely mixed tanks-in-series can be applied as indicated in the following general mass balance formulation of one such tank:

$$\frac{d(vc)}{dt} = Q_{in} C_{in} - (Q_{out} + Q_{wd} + ET.A).C - rV$$

$$Q_{out} = \alpha h^\beta$$

Where

- V volume of the tank [m^3]
- C_{in} inflow concentration [$g \cdot m^{-3}$]
- C outflow concentration [$g \cdot m^{-3}$]
- Q_{in} inflow rate [$m^3 \cdot d^{-1}$]
- Q_{out} outflow rate [$m^3 \cdot d^{-1}$]
- Q_{wd} rate of water withdrawal from the tank [$m^3 \cdot d^{-1}$]
- ET water loss by evapotranspiration [$m \cdot d^{-1}$]
- A surface area of the river tank [m^2]
- r reaction rate [$g \cdot m^{-3} \cdot d^{-1}$]

h hydraulic depth at a time t for rectangular cross-section [m] = V/A
 β, α parameters estimated from stage flow relations
 t simulation time step [d]

Dynamic modeling serially connected with CSTRs such that it can be assumed to represent the behavior of a river stream. Each reactor forms a computational element and then connected sequentially to similar elements upstream and downstream.

These following assumptions were used for the model development:

- Well-mixed dendritic stream.
- Well mixing in cross sections of the river.
- Constant stream flow and channel cross section.
- Constant chemical and biological reaction rates within the computational element.
- The water loss due to upstream fresh water abstraction was not considered explicitly in the water balance.

All of physical, chemical and biological reactions and interactions that might occur in the stream have been considered. The modelling strategy in this study related to QUAL2E water quality model (Brown and Barnwel, [2, 16]; Yuceer et al., [14]). Organic nitrogen, ammonia nitrogen, nitrate nitrogen, nitrite nitrogen, biological oxygen demand, dissolved oxygen, organic phosphorous, dissolved phosphorus, chloride, coliforms, and phytoplanktonic algae which presented as the representative elements of water quality from the perspective of environmental pollution are considered as constituents. The mass balances for these constituents were written and additionally several algebraic equations as mathematical model used to describe various phenomena such as conversion of different forms of nitrogen (as shown in Fig. 1) were involved. Thus the model simulates stream flow and 11 water quality constituents, i.e. state variables.

THE MODEL

Descriptive equations for the properties and constituents considered were established by considering a volume element of the stream as follows:

Ammonia nitrogen:

$$\frac{dN_1}{dt} = \beta_3 \cdot N_4 - \beta_1 \cdot N_1 + \frac{\sigma_3}{d} - F_1 \cdot \alpha_1 \cdot \mu \cdot A + (N_1^0 - N_1) \cdot \frac{Q}{V} + \text{ET.A.N}_1 \quad (1)$$

where F_1 is given by ,

$$F_1 = \frac{P_N \cdot N_1}{(P_N \cdot N_1 + (1 - P_N) \cdot N_3)} \quad (2)$$

Nitrite nitrogen:

$$\frac{dN_2}{dt} = \beta_1 \cdot N_1 - \beta_2 \cdot N_2 + (N_2^0 - N_2) \cdot \frac{Q}{V} + ET.A.N_2 \quad (3)$$

Nitrate nitrogen:

$$\begin{aligned} \frac{dN_3}{dt} = \beta_2 \cdot N_2 - (1 - F_1) \cdot \alpha_1 \cdot \mu \cdot A \\ + (N_3^0 - N_3) \cdot \frac{Q}{V} + ET.A.N_3 \end{aligned} \quad (4)$$

Organic nitrogen:

$$\begin{aligned} \frac{dN_4}{dt} = \alpha_1 \cdot \rho \cdot A - \beta_3 \cdot N_4 \\ - \sigma_4 \cdot N_4 (N_4^0 - N_4) \cdot \frac{Q}{V} + ET.A.N_4 \end{aligned} \quad (5)$$

Rate correction factors for oxidation of ammonia and nitrite:

$$C_{ORDO} = 1.0 - \exp(-K_{NITRF} \cdot DO) \quad (6)$$

$$\text{Ammonia; } (\beta_1) \text{ inhibition} = C_{ORDO} \cdot (\beta_1) \text{input} \quad (7)$$

$$\text{Nitrite; } (\beta_2) \text{ inhibition} = C_{ORDO} \cdot (\beta_2) \text{input.} \quad (8)$$

Organic phosphorus:

$$\begin{aligned} \frac{dP_1}{dt} = \alpha_2 \cdot \rho \cdot A - \beta_4 \cdot P_1 - \sigma_5 \cdot P_1 (P_1^0 - P_1) \cdot \frac{Q}{V} \\ + ET.A.P_1 \end{aligned} \quad (9)$$

Dissolved phosphorus:

$$\begin{aligned} \frac{dP_2}{dt} = \beta_4 \cdot P_1 + \frac{\sigma_2}{d} - \alpha_2 \cdot \mu \cdot A + (P_2^0 - P_2) \cdot \frac{Q}{V} \\ + ET.A.P_2 \end{aligned} \quad (10)$$

Carbonaceous BOD:

$$\frac{dL}{dt} = -K_1 \cdot L - K_3 \cdot L + (L^0 - L) \cdot \frac{Q}{V} + ET.A.L \quad (11)$$

Dissolved oxygen:

$$\frac{dO}{dt} = K_2 \cdot (O^* - O) + (\alpha_3 \cdot \mu - \alpha_4 \cdot \rho) \cdot A - K_1 \cdot L - \frac{K_4}{d} - \alpha_5 \cdot \beta_1 \cdot N_1 - \alpha_6 \cdot \beta_2 \cdot N_2 + (O^0 - O) \cdot \frac{Q}{V} + ET.A.O \quad (12)$$

Then the predictive equation for the saturation (equilibrium) concentration of dissolved oxygen is given below [5]:

$$\begin{aligned} \ln O^* = -139.34410 + \left(\frac{1.575701105}{T} \right) - \left(\frac{6.642308107}{T^2} \right) \\ + \left(\frac{1.2438001010}{T^3} \right) - \left(\frac{8.6219491011}{T^4} \right) \end{aligned} \quad (13)$$

where T is the temperature as K .

For non-standard conditions of pressure, the equilibrium concentration of dissolved oxygen is corrected by this following equation (5)

$$O_P = O^* \cdot P \cdot \left[\frac{(1 - P_{WW}/P) \cdot (1 - \theta \cdot P)}{(-P_{WW}) \cdot (1 - \theta)} \right] \quad (14)$$

$$\ln P_{WW} = 11.8571 - (3840.70/T) - (216961/T^2) \quad (15)$$

$$\theta = 0.000975 - (1.426 \times 10^{-5} \cdot T) + (6.436 \times 10^{-8} \cdot T) \quad (16)$$

where T is $^{\circ}\text{C}$.

Coliforms:

$$\frac{dE}{dt} = -K_5 \cdot E + (E^0 - E) \cdot \frac{Q}{V} + ET \cdot A \cdot E \quad (17)$$

Arbitrary nonconservative constituent: As for the non-conservative constituent, we have chosen chloride

$$\frac{dR}{dt} = -K_6 \cdot R - \sigma_6 \cdot R + \frac{\sigma_7}{d} + (R^0 - R) \cdot \frac{Q}{V} + ET \cdot A \cdot R \quad (18)$$

Phytoplanktonic algae (Chlorophyll a):

$$\frac{dA}{dt} = \mu \cdot A - \rho \cdot A - \frac{\sigma_1}{d} \cdot A + (A^0 - A) \cdot \frac{Q}{V} \quad (19)$$

Algal specific growth rate:

$$\mu = \mu_{\max} (FL) \cdot \left[\frac{2}{1/FN + 1/FP} \right] \quad (20)$$

Algal-light relationships:

$$F_L = \left(\frac{1}{\lambda \cdot d} \right) \ln \left[\frac{K_L + I}{K_L + I \cdot e^{\lambda \cdot d}} \right] \quad (21)$$

Algal self shading:

$$\lambda = \lambda_0 + \lambda_1 \cdot \alpha_0 \cdot A + \lambda_2 \cdot (\alpha_0 \cdot A)^{2/3} \quad (22)$$

Then, the algal growth limitation factors for nitrogen (F_N) and for phosphorus (F_P) are defined by the Monod Expressions as follows:

$$F_N = \frac{N_e}{N_e + K_N} \quad (23)$$

$$F_P = \frac{P_2}{P_2 + K_P} \quad (24)$$

Algae are assumed to use ammonia and/or nitrate as a source of inorganic nitrogen (polluted sources). The effective concentration of available nitrogen is given by:

$$N_e = N_1 + N_3 \quad (25)$$

Notation used for the above equations:

A	Algal biomass concentration, mg-A/L
C	Concentration, (mg/L)
C_{ORDO}	Nitrification rate correction factor
d	Mean stream depth, m
F_1	Fraction of algal nitrogen uptake from ammonia pool
F_L	Algal growth limitation factor for light
F_N	Algal growth limitation factor for nitrogen
F_P	Algal growth limitation factor for phosphorus
I	Surface light intensity, Cal/m ² -hr
K_1	BOD deoxygeneration rate constant, 1/day
K_2	Reaeration rate constant, 1/day
K_3	Rate of loss of BOD due to settling, 1/day
K_4	Benthic oxygen uptake, mg-O/m ² -day
K_5	Coliform die-off rate, 1/day
K_6	Arbitrary non-conservative decay coefficient, 1/day
K_L	Half saturation coefficient for light, Cal/m ² -hr
K_N	The Michaelis Menten half-saturation constant for nitrogen, mg-N/L
K_{NITRF}	First order nitrification inhibition coefficient, mg/L
K_P	The Michaelis Menten half-saturation constant for phosphorus, mg-P/L
L	Concentration of ultimate carbonaceous BOD, mg/L
N_1	Ammonia nitrogen concentration, mg-N/L
N_2	Nitrite nitrogen concentration, mg-N/L
N_3	Nitrate nitrogen concentration, mg-N/L
N_4	Organic nitrogen concentration, mg-N/L
N_e	The effective local concentration of available inorganic nitrogen, mg-N/L
O^*	The saturation concentration of dissolved oxygen at the local temperature and pressure, mg/L
O	The concentration of dissolved oxygen, mg/L
P_2	The local concentration of dissolved phosphorus, mg-P/L
P_N	Preference factor for ammonia nitrogen
P_{ww}	Partial pressure of water vapor, atm
Q	Flow rate, m ³ /s
t	Time, day
T	Temperature, K
V	Volume of water in each divided CSTR, m ³
α_0	Conversion factor; ratio of chlorophyll-A to algal biomass, ug-Chl a/mg-A
α_1	Fraction of algal biomass that is nitrogen, mg-N/mg-A
α_2	Fraction of algal biomass that is phosphorous, mg-P/mg-A
α_3	O ₂ production per unit of algal growth, mg-O/mg-A
α_4	O ₂ uptake per unit of algae respired, mg-O/mg-A
α_5	O ₂ uptake per unit of NH ₃ oxidation, mg-O/mg-N
α_6	O ₂ uptake per unit of NO ₂ oxidation, mg-O/mg-N
β_1	Rate constant for the biological oxidation of NH ₃ to NO ₂ , 1/day
β_2	Rate constant for the biological oxidation of NO ₂ to NO ₃ , 1/day
β_3	Rate constant for the hydrolysis of organic N to ammonia, 1/day

β_4	Rate constant for the decay of organic-P to dissolved-P, 1/day
σ_1	Algal settling rate, m/day
σ_2	Benthos source rate for dissolved phosphorus, mg-P/m ² -day
σ_3	Benthos source rate for ammonia nitrogen, mg-N/m ² -day
σ_4	Organic nitrogen settling rate, 1/day
σ_5	Organic phosphorus settling rate, 1/day
σ_6	Arbitrary non-conservative settling rate, 1/day
σ_7	Benthos source rate for arbitrary non-conservative settling rate, mg-ANC/m ² -day
λ	Light extinction coefficient, m ⁻¹
σ_0	Non-algal portion of the light extinction coefficient, m ⁻¹
σ_1	Linear algal self shading coefficient, m ⁻¹ (ug-Chla/L) ⁻¹
σ_2	Nonlinear algal self shading coefficient, m ⁻¹ (ug-Chla/L) ^{-2/3}
ρ	The local respiration rate of algae, 1/day
μ	The local specific growth rate of algae, 1/day
μ_{\max}	Maximum specific algal growth rate, 1/day

CONCLUSIONS

This paper presents model for river water model based on the mass balance and CSTR approach. The evaporation factor then included in this model. From the explanation above, can be concluded that high rates of water withdrawal at the upstream point can cause an increase in total dissolved solid (TDS) concentration in the downstream reaches of the river.

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