C Program for River Water-Quality Nitrogen Model

Najmussahar H Mulla[1] Dr. B. M. Krishna[2] Dr. B. Manoj Kumar[3] Mudassira Tahneet B. Lahori[4]
[1]M. Tech Scholar [2]Associate Professor [3]Professor [4]Assistant Professor
[1,2,3]Department of Environmental Engineering [4]Department of Computer Science and Engineering
[1,2,3]Sri Jayachamrajendra College of Engineering, Mysore-570006, India [4]Bearys Institute of Technology, Mangalore-574153, India

Abstract— Water is essential for life on Earth, and any changes in the natural quality and distribution of water have ecological impacts that can be threatening. Water quality management is a critical component of overall integrated water resources management. Water resources management involves the monitoring and management of water quality as much as the monitoring and management of water quantity. Water quality models can be effective tools to simulate and predict pollutant transport in water environment and moreover they serve as a base for environmental management decisions. Nitrogen if present in adequate quantities can be used to meet the biochemical requirements of the organisms otherwise can become critical component of eutrophication and hence become integral part of water-quality modeling. This paper is devoted to development of C program for existing nitrification model.

Key words: Nitrification, Denitrification, Eutrophication, Dissolved Oxygen, Modeling

I. Introduction

Water is essential for life on Earth, and any changes in the natural quality and distribution of water have ecological impacts that can be threatening. Rivers serve multifarious water use needs such as irrigation, power generation, navigation, recreation, waste disposal, fish and wild life habitat, etc. The human activity generated contamination from agricultural, municipal and industrial activities introduces significant amount of nutrients and organic materials into the rivers and streams. Discharge of degradable wastewater in the rivers result in a decrease in dissolved oxygen concentrations. Nitrogen compounds are referred to as nutrients because they are essential to life processes of aquatic organisms. Nitrogen is important in water quality modeling for reasons other than its role as a nutrient. For example, the oxidation of ammonia to nitrate during the nitrification process consumes oxygen and may represent a significant portion of the total BOD. Also, high concentrations of unionized ammonia can be toxic to fish and other aquatic organisms. The main objective of this paper is to develop C programs for the existing nitrification model which is developed by Steven C. Chapra . Four C programs are developed for nitrogen species namely ammonia nitrogen, organic nitrogen, nitrite nitrogen and nitrate nitrogen. Algorithms are designed for all C programs developed and given in the paper.

Any natural body of water may be viewed as a system composed of a number of complex interacting subsystems each having its own unique characteristics. For convenience, the system is categorized as physical, chemical and biological components involving many factors and processes that may be interacting with one another. From an engineering point of view, the system may best be described in a mathematical frame work, such that for each of the physical characteristics there may be a written mathematical statement which bears a one- to-one correspondence to it.

A mathematical model is defined as an idealized formulation that represents the response of physical system to external stimuli. The use of models is becoming an integral part of the water quality management process. The use of the computer for the simulation of water-related processes has made water quality-modeling a relatively inexpensive tool to investigate the impact of alternative development approaches before any irreversible action is taken.

II. Nitrogen

A. General

"Fig. 1," depicts the nitrogen cycle in natural waters. As can be seen the cycle affects the water's oxygen level. In addition several other water-quality problems occur. The problems can be grouped into two categories. In the first group are nitrification, denitrification and eutrophication. For these problems nitrogen serves as the cause of the problem rather than as a problem in itself. In the second group are nitrate pollution and ammonia toxicity. In these cases nitrogen species are the actual pollutants.

B. Nitrification/Denitrification

Ammonia due to direct loadings and to the decomposition of organic nitrogen is oxidized in a two-step process to form nitrite (NO2) and nitrate (NO3). If conditions go anaerobic the nitrate can be reduced to nitrite and the nitrite converted to free nitrogen by denitrification.

C. Eutrophication

Aside from its other characteristics, nitrogen serves as an essential nutrient for plant growth. Thus it acts as a fertilizer that can over stimulate plant growth in the process called eutrophication.

D. Nitrate Pollution

The ultimate result of the nitrification process is nitrate. The problem can become especially critical in agricultural regions where nonpoint sources of nitrate from fertilization supplement high levels due to nitrification from point sources.

E. Ammonia Toxicity

Ammonia exists in two forms in natural waters: ammonium ion (NH4) and ammonia gas (NH3). Whereas the former is innocuous at the levels encountered in most natural waters, the un-ionized form is toxic to fish. The equilibrium relationship between the two forms is governed primarily by pH. At high pH (and to a lesser extent at high temperatures), ammonia exists principally in the toxic, un-ionized form.

III. REACTIONS

The conversion of ammonia to nitrate is collectively called nitrification. It can be represented by a series of reactions (Gaudy and Gaudy 1980). In the first, bacteria of the genus Nitrosomonas convert ammonium ion (NH_4^+) to nitrite "(1.1)."

In the second, bacteria of the genus Nitrobacter convert nitrite to nitrate "(1.2)."

$$NH_4^+ + 1.5O_2 \longrightarrow 2H^+ + H_2O + NO_2^- \quad (1.1)$$

$$NO_2^- + 0.5O_2 \longrightarrow NO_3^- \quad (1.2)$$

The oxygen consumed in the two stages can be computed as:

$$r_{oa} = \frac{1.5(32)}{14} = 3.43\ gO\ gN^{-1} \quad (1.3)$$

$$r_{oi} = \frac{0.5(32)}{14} = 1.14\ gO\ gN^{-1} \quad (1.4)$$

$$r_{on} = r_{oa} + r_{oi} = 4.57\ gO\ gN^{-1} \quad (1.5)$$

Where r_{oa} and r_{oi} represent the amount of oxygen consumed due to nitrification of ammonium and nitrite, respectively. r_{on} represent the amount of oxygen consumed per unit mass of nitrogen oxidized in the total process of nitrification.

IV. EQUATIONS

A. Oxygen Deficit Balance (D):

$$\frac{dD}{dt} = r_{oa}\,k_{ai}N_a + r_{oi}k_{in}N_i - k_aD \quad (1.6)$$

B. Organic Nitrogen (N_o):

$$N_o = N_{oO}e^{-k_{oa}t} \quad (1.7)$$

C. Ammonia Nitrogen (N_a):

$$N_a = N_{aO}e^{-k_{ai}t} + \frac{k_{oa}N_{oO}}{k_{ai}-k_{oa}}\left(e^{-k_{oa}t} - e^{-k_{ai}t}\right) \quad (1.8)$$

D. Nitrite Nitrogen (N_i):

$$N_i = \frac{k_{ai}N_{aO}}{k_{in}-k_{ai}}\left(e^{-k_{ai}t} - e^{-k_{in}t}\right) + \frac{k_{ai}k_{oa}N_{oO}}{k_{ai}-k_{oa}} * \left(\frac{e^{-k_{oa}t}-e^{-k_{in}t}}{k_{in}-k_{oa}} - \frac{e^{-k_{ai}t}-e^{-k_{in}t}}{k_{in}-k_{ai}}\right) \quad (1.9)$$

E. Nitrate Nitrogen (N_n):

$$N_n = +N_{aO} - N_{oO}e^{-k_{oa}t} - N_{aO}e^{-k_{ai}t} - \frac{k_{oa}N_{oO}}{k_{ai}-k_{oa}} * \left(e^{-k_{oa}t} - e^{-k_{ai}t}\right) - \frac{k_{ai}N_{aO}}{k_{in}-k_{ai}}\left(e^{-k_{ai}t} - e^{-k_{in}t}\right) - \frac{k_{ai}k_{oa}N_{oO}}{k_{ai}-k_{oa}}\left(\frac{e^{-k_{oa}t}-e^{-k_{in}t}}{k_{in}-k_{oa}} - \frac{e^{-k_{ai}t}-e^{-k_{in}t}}{k_{in}-k_{ai}}\right) \quad (1.10)$$

Where $N_o = N_{oO}$ and $N_a = N_{aO}$ at $t = 0$ and k_{ai}, k_{oa}, k_{in} are first order rate constants.

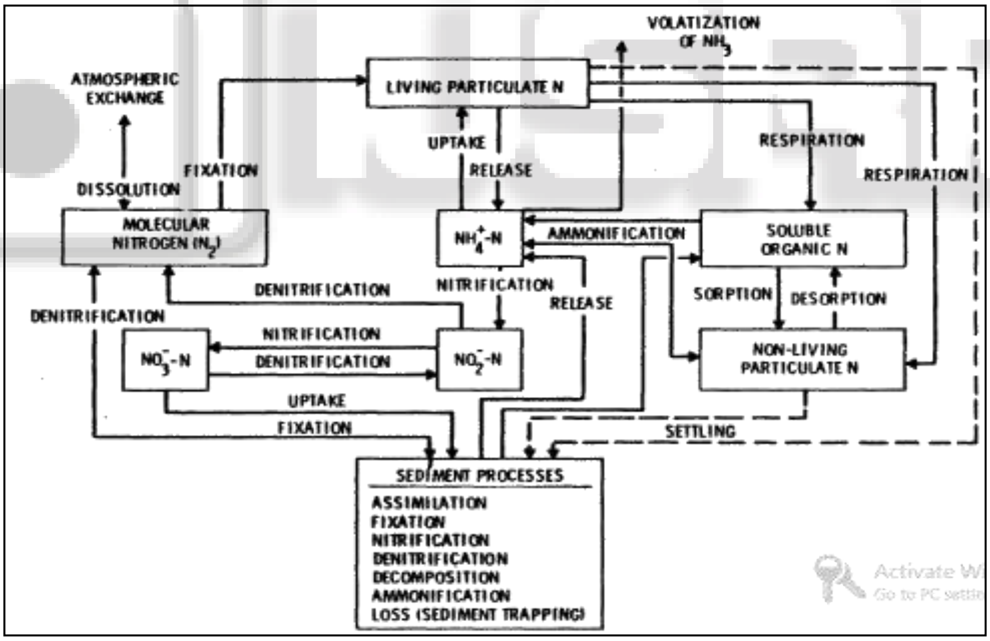

Fig. 1: Nitrogen Cycle and Processes Related To Nitrogen Modeling

V. ALGORITHMS

A. Organic Nitrogen:

1) STEP 1: START
2) STEP 2: INPUT **N_{oO}, k_{oa}, t**
   (IF NO VALUES AVAILABLE INPUT ZERO)
3) STEP 3: CALCULATE
   N = ((-k_{oa})*t)
4) STEP 3: CALCULATE
   N_o = (N_{oO}*exp(N))
5) STEP 4: OUTPUT **'N_o'**
6) STEP 5: STOP

B. Ammonia Nitrogen:

1) STEP 1: START
2) STEP 2: INPUT N_{aO}, k_{ai}, N_{oO}, k_{oa}, t
   (IF NO VALUES AVAILABLE INPUT ZERO)
3) STEP 3: CALCULATE
   a = ((-k_{oa})*t)
4) STEP 4: CALCULATE
   b= ((-k_{ai})*t)
5) STEP 5: CALCULATE

c= (exp(a) - exp(b))
6) STEP 6: CALCULATE
$d=k_{ai} - k_{oa}$
7) STEP 7: CALCULATE
$N_a= ((N_{aO}*exp(b)) + (((k_{oa}*N_{oO})/d)*c))$
8) STEP 8: OUTPUT 'N_a'
9) STEP 9: STOP

C. *Nitrite Nitrogen:*

1) STEP 1: START
2) STEP 2: INPUT N_{aO}, k_{ai}, N_{oO}, k_{oa}, k_{in}, t
(IF NO VALUES AVAILABLE INPUT ZERO)
3) STEP 3: CALCULATE
$a = ((-k_{oa})*t)$
4) STEP 4: CALCULATE
$b= ((-k_{ai})*t)$
5) STEP 5: CALCULATE
$c= ((-k_{in})*t)$
6) STEP 6: CALCULATE
$A= ((k_{ai}*N_{aO})/(k_{in}-k_{ai}))$
7) STEP 7: CALCULATE
B= (exp(b)-exp(c))
8) STEP 8: CALCULATE
$C= ((k_{ai}*k_{oa}*N_{oO}) / (k_{ai}-k_{oa}))$
9) STEP 9: CALCULATE
$D= ((exp(a)-exp(c)) / (k_{in}-k_{oa}))$
10) STEP 10: CALCULATE
$E= ((exp(b)-exp(c)) / (k_{in}-k_{ai}))$
11) STEP 11: CALCULATE
Ni= ((A*B) + (C*(D-E)))
12) STEP 12: OUTPUT 'N_i'
13) STEP 13: STOP

D. *Nitrate Nitrogen:*

1) STEP 1: START
2) STEP 2: INPUT N_{aO}, k_{ai}, N_{oO}, k_{oa}, k_{in}, t
(IF NO VALUES AVAILABLE INPUT ZERO)
3) STEP 3: CALCULATE
$a = ((-k_{oa})*t)$
4) STEP 4: CALCULATE
$b= ((-k_{ai})*t)$
5) STEP 5: CALCULATE
$c= ((-k_{in})*t)$
6) STEP 6: CALCULATE
$d= (N_{oO}+N_{aO}-(N_{oO}*exp(a))-(N_{aO}*exp(b)))$
7) STEP 7: CALCULATE
$e= ((k_{oa}*N_{oO})/(k_{ai}-k_{oa}))$
8) STEP 8: CALCULATE
$A= ((k_{ai}*N_{aO})/(k_{in}-k_{ai}))$
9) STEP 9: CALCULATE
B= (exp(b)-exp(c))
10) STEP 10: CALCULATE
$C= ((k_{ai}*k_{oa}*N_{oO}) / (k_{ai}-k_{oa}))$
11) STEP 11: CALCULATE
$D= ((exp(a)-exp(c)) / (k_{in}-k_{oa}))$
12) STEP 12: CALCULATE
$E= ((exp(b)-exp(c)) / (k_{in}-k_{ai}))$
13) STEP 13: CALCULATE
$N_n= (d-(e*(exp(a)-exp(b)))-(A*B)-(C*(D-E)))$
14) STEP 14: OUTPUT 'N_n'
15) STEP 15: STOP

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