MATHEMATICAL MODELING AND ANALYSIS OF AMMONIA, NITRITE, AND NITRATE CONCENTRATION: CASE STUDY IN THE POLDER TAWANG SEMARANG, INDONESIA

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Abstract. In this paper a mathematical model is proposed for a qualitative representative of nitrogen dynamics in the Polder Tawang Water. The model variables are the concentration of ammonia, nitrite, and nitrate. The model consists of three coupled ordinary differential equations. The model was calibrated to field data for the Polder Tawang Water. Further, simulation analysis is performed to find the maximal concentration of nitrogen and the stability of the proposed model. From the simulation results, the nitrite-nitrogen concentration is about 0.038 mg/L. It indicate that Polder Tawang water seriously polluted.

Key words and Phrases : water quality, mathematical modeling, ammonia, nitrite, nitrate.

1. INTRODUCTION

The degradation of water quality in Polder Tawang, located in Semarang, Central Java, Indonesia, has attracted Local Goverment. The functions of the Polder Tawang are to collect the water transfer from the outside area and to control the water surface in the old town. But, the Polder is used by the community for receiving their domestic waste. This condition cause the consentration of a number of pollutants such as nitrogen has increased.

A dynamic nitrogen balanced model for river systems have been developed by Whitehead and Williams [7]. Then, the implementation of, a mathematical framework for inferring optimal patterns of water and nitrogen have discussed by Buckley, et.al.[1]. Their analysis is limited to a time scale of one day and a spatial scale consisting of the green canopy of one plant. Further, the MASONW (MACRO + SOILN + Watershed) model describing nitrogen leaching in watersheds have been developed and tested [8]. While, An accounting for the role of sludge remineralization in the dynamics of N in shrimp ponds makes little difference to the evaluation of management strategies that do not involve manipulation of the sludge N pool [2].

Furthermor, some reseachers [3] studied the dynamics of the gene circuit responsible for regulating nitrogen catabolite represston in yeast. The problems of mathematical modelling of homogeneuos oxidation of nitrogen oxide, wich takes place in different parts of nitric acid production plants have been published by Djambov and Ruseva [5]. A non-linear mathematical model is proposed for a qualitative representation of ecosystem dynamics in a eutrophied water body [6].

In this paper, we propose the mathematical model for ammonia, nitrite, and nitrate concentration dynamics in the Polder Tawang Water. The differential equations system governing transformations in the nitrification process are discussed. Then, simulation results are demonstrated to check the optimal concentration of nitrogen and the stability of the system.

The paper is organized as follows. Section 2 describes the field data collections from the Polder Tawang water. Results concerning mathematical models of ammonia, nitrite, and nitrate are presented in Section 3. In Section 4 the simulation results of the calibration of the models are demonstrated . Finally, concluding remarks are drawn in Section 5.

2. DATA COLLECTION

We consider here the Polder Tawang water which is being polluted. For mathematical modeling, we take the water sample from three locations in the Polder Tawang, i.e. near right filtration, middle, and near left filtration, about 1,5 L for each station and in the depth about 1 m (is below water surface). Nitrogen concentration measurement consists of ammonia (NH_3), nitrite (NO_2), and nitrate (NO_3) concentration. Those mesurements are done in the Chemical Laboratory. Whereas, PH, temperature, salinity, and turbidity measurements are directly done in the Polder Tawang. The field measurement results of ammonia,

Treatment	Sample Code	NH3 (mg/L)	NO2 (mg/L)	NO3 (mg/L)
I	A1	31.83	0.023	1.9
	B1	24.72	0.007	1.18
	C1	35.51	0.003	2.54
II	A2	23.23	0.008	0.81
	B2	19.41	0.018	0.72
	C2	18.42	0.031	0.81
III	A3	25.22	0.023	1.62
	B3	21.24	0.007	1.62
	C3	23.39	0.003	1.7
IV	A4	19.31	0.009	1.62
	B4	21.7	0.016	1.47
	C4	20.18	0.004	1.09
V	A5	14.14	0.167	1.5
	B5	11.22	0.013	1.5
	C5	12.54	0.189	1.07

nitrite, and nitrate concentration are given in the Table 1.

Table 1. The field data of ammonia, nitrite, and nitrate concentration

Note: A (right filtration), B (middle), C (left filtaration)

The average values of ammonia are depicted in Figure 1. From this figure, it can be seen that average value distributions of ammonia-nitrogen concentration in the Polder Tawang achieve between 19,66 – 22,75 mg/L. Whereas, the average ammonia-nitrogen concentration from results measurement in the near right filtration, meddle, and near left filtration is 21,47 mg/L. The average value of ammonia concentartion from near right filtration is highest (see Figure 1).

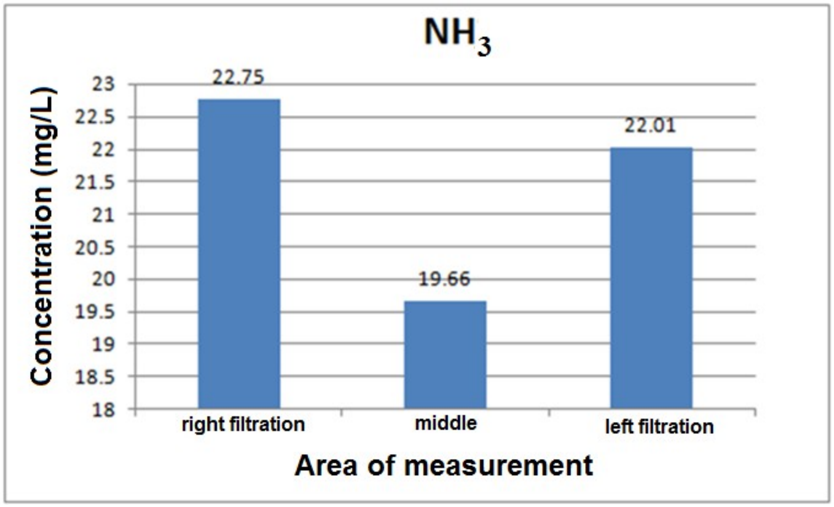

Figure 1. The average values of ammonia

The average values of nitrite-nitrogen are given in Figure 2. In Figure 2, we see that average value distributions of nitrite-nitrogen concentration achieve between 0,012 – 0,046 mg/L with the totality of average

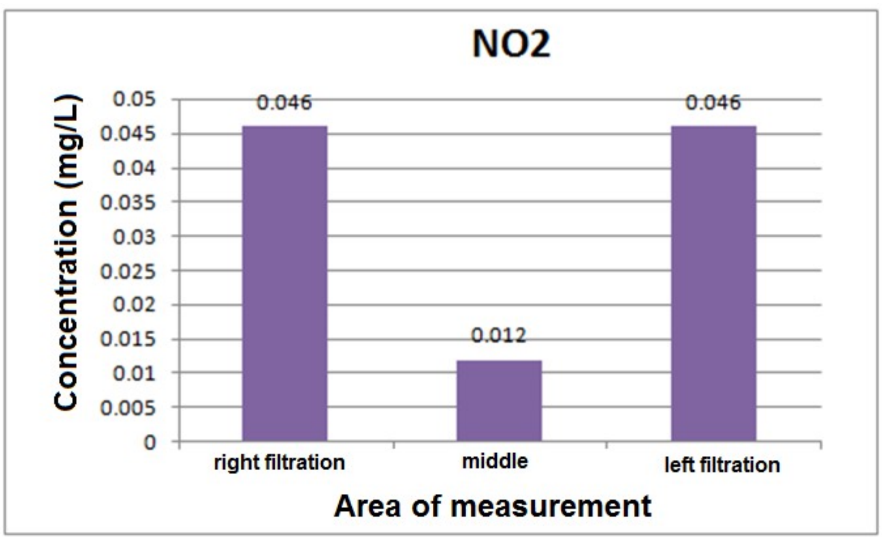

Figure 2. The average values of nitrite

Nitrite (NO_2)-nitrogen concentration in the near right filtration, middle, and near left filtration is 0,035 mg/L.

The average values of NO_3 are shown in Figure 3. From this figure, it can be seen that average value distributions of NO_3-nitrogen concentration in the Polder Tawang achieve between 1,3 – 1,49 mg/L. Whereas, the average nitrate-nitrogen concentration from results measurement in the near right filtration, meddle, and near left filtration is 1,41 mg/L.

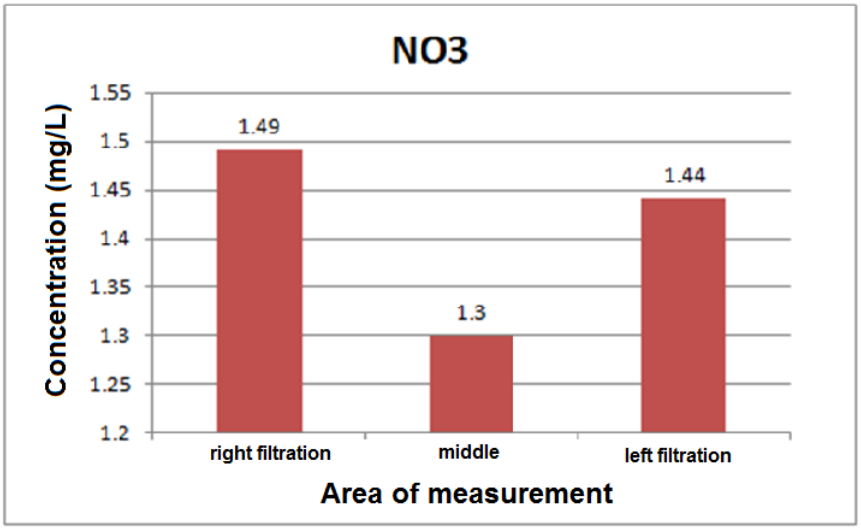

Figure 3. The average values of ammonia

The average value of nitrate concentartion from near right filtration is highest (see Figure 3). The condition of water quality based on the nitrite-nitrogen concentration is given in Table 2.

Table 2. Water quality based on Nitrite concentration

No	Nitrite concentration (mg/L)	Condition of Water quality
1	< 0,003	No polluted - little polluted
2	0,003 – 0,014	Medium polluted
3	0,014 – 0,10	Seriously polluted

The water quality data of Polder tawang corresponding to temperature, PH, turbidity, and salinity are as follows. Temperature = 31^0 C, PH = 8, turbidity = 73.4 %, and salinity = 0. From the measurement results, it is found that the PH of the Polder Tawang water is base.

3. MATHEMATICAL MODELING

Most modeling studies have been restricted to the nitrification process since the discharge of nitrogen into water bodies from industrial or domestic effluents has a significant effect on water quality, fisheries, as indicated in the following equations, dissolved oxygen levels [7].

$$NH_4^+ + \frac{3}{2}O_2 \xrightarrow{\text{Nitrosomonas}} 2H^+ + H_2O + NO_2^-$$
$$NO_2^- + \frac{1}{2}O_2 \xrightarrow{\text{Nitrobacter}} NO_3^- \qquad (1)$$

Nitrosomas and Nitrobacter are autotrophic bacteria responsible for the oxidation process. The differential equations governing transformations of nitrogen from one from an other (1) of the nitrification process first-order reaction are given below[4].

$$\frac{d}{dt}N_1(t) = -k_1 N_1(t),$$
$$\frac{d}{dt}N_2(t) = k_1 N_1(t) - k_2 N_2(t),$$
$$\frac{d}{dt}N_3(t) = k_2 N_2(t), \tag{2}$$

where

$$N_1(0) \geq 0,\ N_2(0) \geq 0,\ N_3(0) \geq 0.$$

Here N_1 is ammonia-nitrogen concentration, N_2 is nitrite-nitrogen concen-tration, N_3 is nitrate-nitrogen concentration, t is time, k_1 and k_2 are rate constant for the oxidation of ammonia-nitrogen and rate constant for the oxidation of nitrite-nitrogen respectively.

By solving the differential equation systems(2), we find the model of the concentration nitrogen as follows

$$N_1(t) = \frac{767}{25} e^{(-k_1 t)},$$
$$N_2(t) = \frac{1}{100}\frac{(30691\ \ k_1 - 11k_2)}{k_1 - k_2} - \frac{767}{25}\frac{k_1 e^{(-k_1 t)}}{k_1 - k_2},$$
$$N_3(t) = -\Bigg(-\frac{767}{25}e^{(-k_1 t)}k_2 + \frac{1}{1000}\frac{e^{(-k_2 t)}(30691\ \ k_1 - 11k_2)k_1}{k_1 - k_2} - \frac{1}{1000}\frac{e^{(-k_2 t)}(30691\ \ k_1 - 11k_2)k_2}{k_1 - k_2} - \frac{32561\ \ k_1}{1000} + \frac{32561\ \ k_1}{1000}\Bigg)\cdot (k_1 - k_2)^{-1}. \tag{3}$$

Further, we will look for an optimal concentration of nitrogen. One method for doing this is based on the derivation that (equation 3). We find that the optimal concentration of nitrite-nitrogen (N_2) occurs at time,

$$t = -\frac{\ln\left(\frac{1}{30680}\frac{30691\ \ k_1 - 11k_2}{k_1^2}\right)}{k_1 - k_2}.$$

Consider that from equation (3), we have

$$\frac{dN_1(t)}{dt} + \frac{dN_2(t)}{dt} + \frac{dN_3(t)}{dt} = 0. \tag{4}$$

The above equation (4) indicate that

$$N_1(t) + N_2(t) + N_3(t) = C, \tag{5}$$

where C is arbitrary constant.

To analysis the stability behaviour of the nitrogen in the phase-plane, we reduce three coupled differential equations (2) into two coupled differential equations by using equation (5).

4. SIMULATION RESULTS

In this section, simulation results are demonstrated to check the optimal concentration of nitrogen and the stability of the system. We conduct some numerical computation by using the data of ammonia, nitrite, and nitrate concentration in Table 1 and the following values of the initial condition in model (1).

$$N_1(0) = 30.68 \ , \ N_2(0) = 0.011 \ , \ N_3(0) = 1.87 \ .$$

Under the above set of values and by using the least square method, we find the parameters $k_1 = 0.002$ and $k_2 = 1.604$. Then, we substitute these parameters to the equations (3) for evaluating the behaviour of dynamics nitrogen. The NH_3, NO_2, NO_3 concentration changes are given in Figure 4-6.

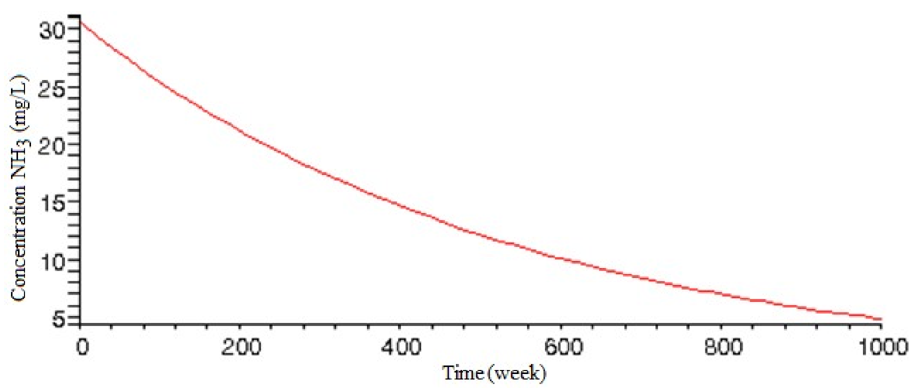

Figure 4. Ammonia concentration vs. Time

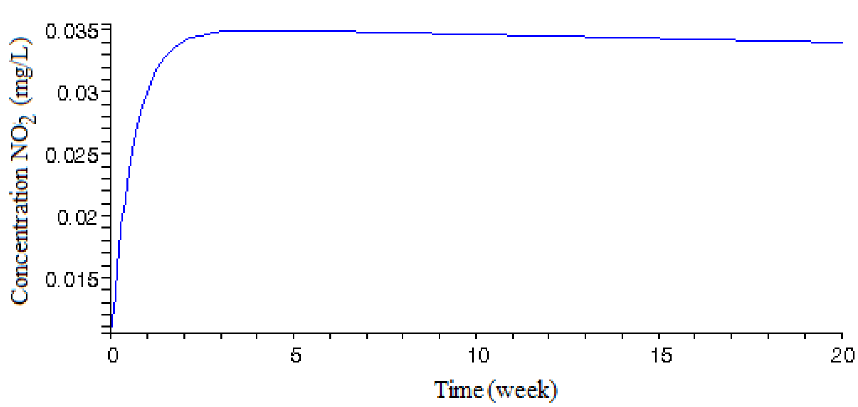

Figure 5. Nitrite concentration vs. Time

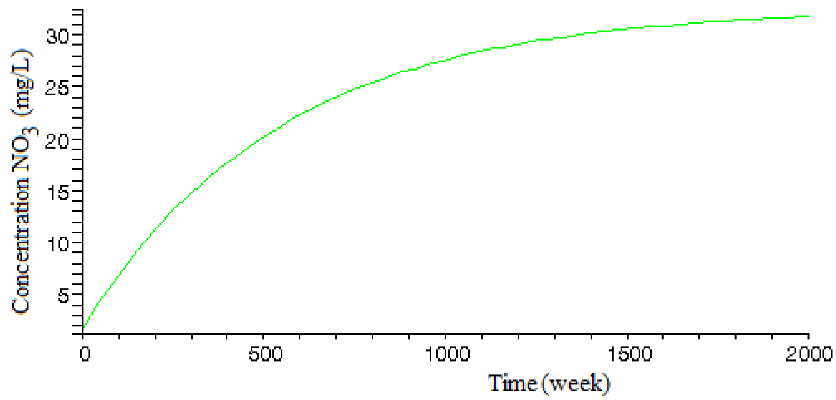

Figure 6. Nitrate concentration vs. Time

From Figure 4-6, we observe here that the concentration of NH_3 will decrease whereas the concentration of NO_3 increases. In these figures we are also seeing that the concentration of NO_2 reaches to its maximum level at 3,96 weeks.
Furthermore, we analyze the stability behaviour of the nitrogen in the phase-plane. The trajectories for the system are depicted in Figure 7-9. For tabouthe above set of parameters, a computer generated graph of N_1 versus N_2 and N_1 versus N_3 are shown in Figure 7-8, which indicate the global stability.

Figure 7 shows that the concentration of ammonia (N_1) will decrease steadily toward a limiting value of 30,2 mg/L whereas the concentration of nitrite (N_2) increase steadily toward a limiting value of 0.038 mg/L. Based on these condition, it is indicated that the Polder Tawang water is seriously polluted.

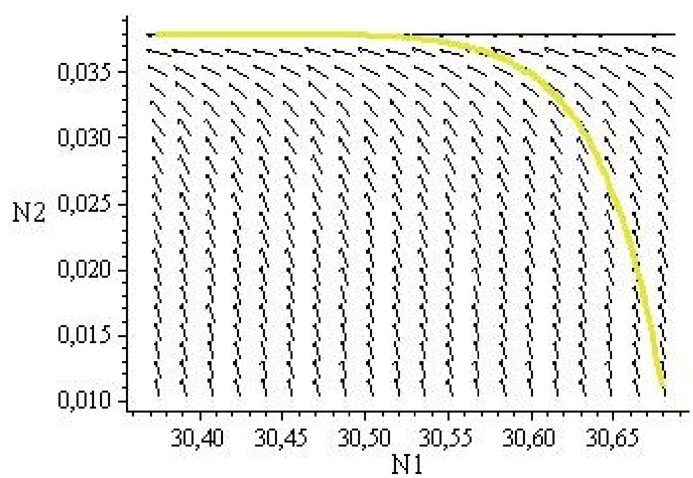

Figure 7. Trajectories for a system in N_1-N_3 plane.

From Figure 8, it can be seen that the concentration of ammonia (N_1) will decrease steadily toward a limiting value of 30,54 mg/L whereas the concentration of nitrate (N_3) increases steadily toward a limiting value of 1.98 mg/L.

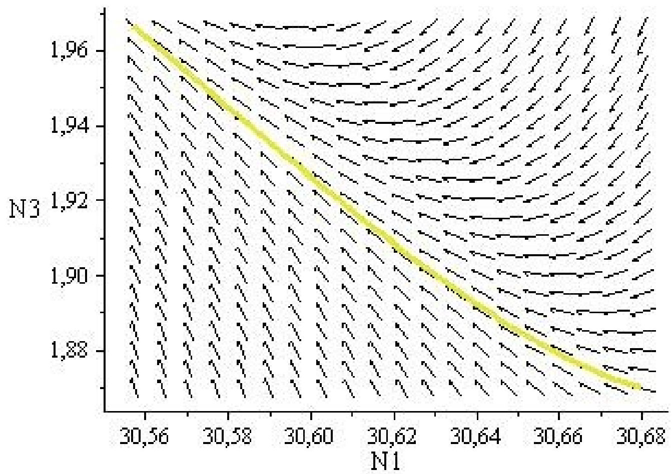

Figure 8. Trajectories for a system in N_1-N_3 plane.

Figure 9 shows that if the concentration of nitrite (N_2) increases, then the concentration of nitrate (N_3) also increases

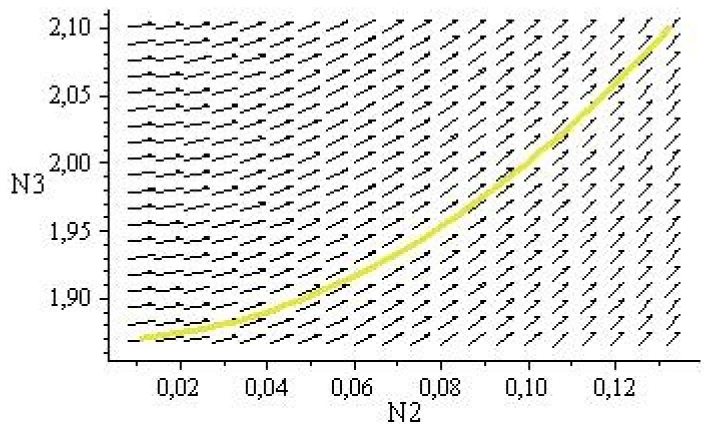

Figure 9. Trajectories for a system in N_2-N_3 plane.

5. CONCLUDING REMARKS

The nitrogen mathematical model has been proposed. By simulation analysis with field data, it has been shown that the trajectories for the system in ammonia-nitrite and ammonia-nitrate plane achieve the global stability. The concentration of nitrite reaches to its maximum level. This maximal value is 0.038 mg/L that occurs at about 3.96

weeks. It has also been shown that the concentration of ammonia decreases, whereas the concentration of nitrite and nitrate increase. Based on the nitrite-nitrogen concentration indicated that the Polder Tawang water seriously polluted.

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REFERENCES

1. T.N. Buckley, J.M. Miller, and G.D. Farquhar, The mathematics of linked optimisation for water and nitrogen use in a canopy, *Silva Fennica* , **36**, 3, 639–669, 2002.
2. M.A. Burford and K. Lorenze, Modeling nitrogen dynamics in intensive shrimp ponds: the role of sediment remineralization, *ELSEVIER: Aquaculture* , **229**, 129–145, 2004.
3. E.M. Boczko, et.al, Structure theorems and the dynamics of nitrogen catabolite repression in yeast, *The National Accademy of Science of the USA,* **102**, 16, 5647-5652, 2005.
4. S. Chapra, *Surface Water Quality Modeling*, Mc Graw-Hill inc., Singapore, 1997.
5. P. Djambov and N. Ruseva, Modelling of nitrogen oxide oxidation in nitric acid production, *Journal of the University of Chemical Technology and Metallurgy,* **41**, 1, 41-44, 2006.
6. A.K. Misra, Mathematical modeling and analysis of eutrophication of water bodies caused by nutrients, *Nonlinear Analysis: Modelling and Control,* **12**, 4, 511-524, 2007.
7. P.G.Whitehead and R.J. Williams, A dynamic nitrogen balanced model for river systems, *IAHS Publ.*, **139**, 89-99, 1982.
8. A. Vassiljev, A. Grimvall and M. Larsson, A dual-porosity model for nitrogen leaching from a watershed, *Hydrological Sciences–Journal–des Sciences Hydrologiques,* **49**, 2, 2004

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