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NITROGEN TRANSFORMATION AND TRANSPORT MODELING IN GROUNDWATER AQUIFERS USING SPREADSHEETS

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ABSTRACT

Groundwater nitrogen pollution is a common problem and it poses a major threat to groundwater-based drinking water supplies. In this study, a kinetic model is developed to study nitrification–denitrification reactions in groundwater aquifers. A new reaction module for the reactive transport in one-dimension code is developed and tested to describe the fate and transport of nitrogen species. The proposed model was developed to simulate groundwater nitrate concentration. The model is later used to study the field-scale nitrogen transport and transformations at a catchment area of Shenyang City. Modeling results are consistent, indicating that the method provides a convenient for solving practical problems on nitrogen transport and transformation. The developed model describing nitrification and denitrification reactions is a useful framework for simulating the fate and transport of nitrogen species in groundwater aquifers.

KEYWORDS: Nitrogen; transportation, transformation; groundwater; modeling; spreadsheets.

1. INTRODUCTION

Groundwater nitrogen pollution is a worldwide problem. In the process of three nitrogen transport, nitrification-denitrification reaction occurs under certain hydrogeochemical condition, thus its concentration changed (Burt et al 2006). At present, there are some difficulties on the quantitative prediction of nitrogen species in the process of its transportation and transformation. The existing commercial groundwater numerical simulation software can simulate the transportation of a variety of components at the same time, but have not provide the coupling of nitrification and denitrification function. Despite some software (such as RT3D, Feflow) accomplished the model secondary development function, but it requires the user must certain computer programing languages. These simulation softwares are highly professional and technical requirements for the users are high, too.

One of the best tools for solving this problem is spreadsheet. One of the best tools for solving the PDE is spreadsheet. There are many advantages of spreadsheets such as having numerical and visual feedback, fast calculating capabilities. One of the most important advantages of spreadsheets is its graphical interface. The solution obtained through the spreadsheet can easily be plotted at the same worksheet. Any changes in the input parameters of the solution domain will be directly reflected to the graphical representation of the solutions. Spreadsheets are user-friendly and easy to program. Several studies have been carried out using spreadsheets for the last 10 years. In this modeling, on a spreadsheet it is not necessary to write out an equation in all cells to carry out iterative calculations. Using copy and paste features of the spreadsheets, the equation can be copied to other cells without writing the equations to all cells individually. When the equation pasted to all cells of the solution domain, iterative calculation is started. It is carried out until the given number of iteration is finished or maximum convergence criterion has been met. The main objective of this study is to develop a user- friendly and flexible method to solve the one-dimensional transport and transformation mathematical model of nitrogen species. (Mee-Sun et al, 1993, Halilkarahan, 2006; Clement, 2001)

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2. MATERIALS AND METHODS

2.1 Nitrogen transformation concept

Mathematical model

2.1. Nitrogen transformations and transport

Ammonium oxidation to nitrite can be written as: (Reddy,1975)

$$NH_4^+ + \frac{3}{2}O_2 \rightarrow NO_2^- + 2H^+ + H_2O \qquad (1)$$

Nitrite oxidation to nitrate can be written as: (Reddy,1975)

$$NO_2^- + \frac{1}{2}O_2 \rightarrow NO_3^- \qquad (2)$$

Dissolved organic carbon is the source of microbial and nitrate reaction, and is assumed to be non-volatile subject to sorption (Jardine et al., 1992). In this paper, the organic compounds are represented by the simplified chemical formula CH_2O, and assumed to be degraded by heterotrophic microorganisms aerobically. When coupled with oxidation of Dissolved organic carbon, the overall reaction for denitrification is:

$$CH_2O + \frac{4}{5}NO_3^- \rightarrow \frac{2}{5}N_2 + \frac{4}{5}HCO_3^- + \frac{1}{5}CO_2 + \frac{1}{5}H_2O \qquad (3)$$

Please note that the dynamic rule between nitrogen species transformation is very complex, a variety of bacteria is the necessary condition to promote the development of the reaction, so it relates to the concentration of bacteria. For this reason, the Eqs. (1)- (3) has to be simplified in the practical work. Generally we believed that the nitrification process could be simplified as a first-order reaction, thus:

The kinetic equations for nitrification have the following form.

NH_4^+ concentration change rate is as follows:

$$-\frac{dC_{N1}}{dt} = K_1 C_{N1} \qquad (4)$$

where K_1 is Eqs.(1) reaction speed constant(T^{-1}).

NO_2^- concentration change rate is as follows:

$$-\frac{dC_{N2}}{dt} = -K_2 C_{N_2} + y_{NO_2/NH_4} K_1 C_{N_1} \qquad (5)$$

where K_2 is Eqs.(2) reaction speed constant(T^{-1}).

NO_3^- concentration change rate is as follows:

$$-\frac{dC_{N3}}{dt} = -K_3 C_{N_3} + y_{NO_3/NO_2} K_2 C_{N_2} \qquad (6)$$

where K_3 is Eqs.(3) reaction speed constant(T^{-1}).

The control equation of transportation and transformation for nitrogen is as follows

$$\frac{\partial[NH_4]}{\partial t} = \frac{D_{L1}\,\partial^2[NH_4]}{R_{NH_4}\,\partial x} - \frac{v\,\partial[NH_4]}{R_{NH_4}\,\partial x} - K_1[NH_4] \qquad (7)$$

$$\frac{\partial[NO_2]}{\partial t} = \frac{D_{L2}\,\partial^2[NO_2]}{R_{NO_2}\,\partial x} - \frac{v\,\partial[NO_2]}{R_{NO_2}\,\partial x} - K_2[NO_2] + y_{NO_2/NH_4} K_1[NH_4] \qquad (8)$$

$$\frac{\partial[NO_3]}{\partial t} = \frac{D_{L3}\,\partial^2[NO_3]}{R_{NO_3}\,\partial x} - \frac{v\,\partial[NO_3]}{R_{NO_3}\,\partial x} - K_3[NO_3] + y_{NO_3/NO_2} K_2[NO_2] \qquad (9)$$

where $[NH_4], [NO_2], [NO_3]$ is the concentration of NH_4^+, NO_2^-, NO_3^-, respectively. $R_{NH_4}, R_{NO_2}, R_{NO_3}$ is the retardation coefficient. v is the infiltration velocity. y_{NO_3/NO_2}, y_{NO_2/NH_4} is the ratio of chemometric number.

With initial and boundary conditions:

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$$\begin{cases} [NH_4](x>0,t=0)=0,[NO_2](x>0,t=0)=0,[NO_3](x>0,t=0)=0; \\ [NH_4](x=0,t\geq 0)=C_0,[NO_2](x=0,t\geq 0)=0,[NO_3](x=0,t\geq 0)=0; \\ [NH_4](x\to\infty,t\geq 0)=0,[NO_2](x\to\infty,t\geq 0)=0,[NO_3](x\to\infty,t\geq 0)=0; \end{cases} \quad (10)$$

$$\begin{cases} \frac{\partial C^1}{\partial t}=\frac{D_{L1}\partial^2 C^1}{R_1\partial x^2}-v\frac{\partial C^1}{R_1\partial x}-K_1C^1 \\ \frac{\partial C^2}{\partial t}=\frac{D_{L2}\partial^2 C^2}{R_2\partial x^2}-v\frac{\partial C^2}{R_2\partial x}-K_2C^2+y_{NO_2/NH_4}K_1C^1 \\ \frac{\partial C^3}{\partial t}=\frac{D_{L3}\partial^2 C^3}{R_3\partial x^2}-v\frac{\partial C^3}{R_3\partial x}-K_3C^3+y_{NO_3/NO_2}K_2C^2 \end{cases} \quad 0\leq x\leq L,\ 0\leq t\leq T, \quad (11)$$

where C_1, C_2, C_3 is the concentration of NH_4^+, NO_2^-, NO_3^- , respectively.
The solution domain of the problem is covered by a mesh of grid-lines
$x_i = i\Delta x$, i = 0, 1, 2,..., M,
$t_n = n\Delta t$, n= 0, 1, 2,..., N,

where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid spacing are $\Delta x=L/M$ and $\Delta t=T/N$.

Consider the following approximations of the derivatives in the advection–diffusion equation which incorporate time and space weights φ and θ as follows [3]:

$$\frac{\partial C}{\partial t}=\frac{c(i,n+1)-c(i,n)}{\Delta t} \quad (12)$$

$$v\frac{\partial c}{\partial x}=(1-\phi)\left\{\frac{v}{\Delta x}[(1-\theta)c(i,n)+\theta c(i+i,n)-(1-\theta)c(i-1,n)-\theta c(i,n)]\right\}+\phi\left\{\frac{v}{\Delta x}[(1-\theta)c(i,n+1)+\theta c(i+1,n+1)-(1-\theta)c(i-i,n+1)-\theta c(i,n+1)]\right\} \quad (13)$$

$$D\frac{\partial^2 c}{\partial x^2}=(1-\phi)\left\{\frac{D}{(\Delta x)^2}[c(i-1,n)-2c(i,n)+c(i+1,n)]\right\}+\phi\left\{\frac{D}{(\Delta x)^2}[c(i-1,n+1)-2c(i,n+1)+c(i+1,n+1)]\right\} \quad (14)$$

where φ is a time weighting factor and θ is the spatial weighting factor.
Substituting Eqs. (12), (13) and (14) into Eq. (11)

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$$A_k c^k(i-1,n+1) + B_k c^k(i,n+1) + C_k c^k(i+1,n+1) = f_k(i,n) \quad (15)$$

where

$$A_k = \left[\phi\left(\frac{Cr_k}{Pe_k}\right) + \phi E Cr_k\right]/R_k \quad (16)$$

$$B_k = \frac{\left[-2\phi\left(\frac{Cr_k}{Pe_k}\right) - \phi(1-2\theta)Cr_k\right]}{R_k} - 1 \quad (17)$$

$$C_k = \left[\phi\left(\frac{Cr_k}{Pe_k}\right) - \phi\theta Cr_k\right]/R_k \quad (18)$$

$$f_k = -c^k(i,n) - \frac{d\left(\frac{Cr_k}{Pe_k}\right)\left[c^k(i+1,n) + c^k(i-1,n) - 2c^k(i,n)\right]}{R_k} + \frac{dCr_k\left[\theta c^k(i+1,n) - Ec^k(i-1,n) + Ec^k(i,n) - \theta c^k(i,n)\right]}{R_k} + K_k c^k \Delta t - K_{k-1} c^{k-1} \Delta t \quad (19)$$

k=1,2,3

d=1-φ

E=1-θ

K_0=0

$$Cr_k = \frac{v_k \Delta t}{\Delta x}$$

$$Pe_k = \frac{v_k \Delta x}{D_k}$$

One equation of the form of (15) is written for each active node, leading to a system of linear algebraic equations. Note that the unknown concentration at any node at the new time level depends on the concentrations at adjacent nodes at the new time level, which are also unknown. Thus, the system of linear algebraic equations resulting from the implicit scheme must be solved simultaneously, using a direct matrix solution technique or an iterative solution method.

This study uses iterative spreadsheet solution as

$$c^k(i,n+1) = \left[f_k(i,n) - A_k c^k(i-1,n+1) - C_k c^k(i+1,n+1)\right]/B_k \quad (20)$$

The solution of Eq. (11) is further analyzed as:
For φ= 1 and θ=1⁄2, Eq. (15) yields the implicit BTCS (Backward time centred space) - type finite difference technique

$$2R_k c^k(i,n) = 2R_k M - \left[2\left(\frac{Cr_k}{Pe_k}\right) + Cr_k\right]c^k(i-1,n+1) - \left[2\left(\frac{Cr_k}{Pe_k}\right) - Cr_k\right]c^k(i+1,n+1) + 2\left[2\left(\frac{Cr_k}{Pe_k}\right) + R_k\right]c^k(i,n+1) \quad (21)$$

Note that it is used for the spatial derivative in the advection term, the backward-difference form for the time derivative and the centered-difference for the spatial derivative in the diffusion term. Eq. (21) is only first-order accurate and incorporates numerical diffusion amounting to $v_k\Delta x/2$.

Similarly, for φ= 1 and θ=0, Eq. (15) may be written as the upwind-type finite difference formula and for φ= 1/2 and θ=1/2, Eq. (5) may be written as the Crank–Nicolson type formula. To eliminate the numerical oscillations and dispersion more efficiently, need to meet, Pe<2; Cr<1; $\Delta x < \alpha_L$ (Lindstrom et al, 1992). This study was within the range.

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Model development

The model implementation is divided into rectangular grid intervals both in x direction and time dimension in order to carry out the iterative spreadsheet calculations (see Fig. 1). In order to achieve the iterative calculations, the maximum number of iterations and maximum error value need to be set be before simulations("Office"-

"Excel Options"-"formula"-"iteration count"). In this study, we set 1000 and 0.0001, respectively.
It takes R_1, R_2, R_3, D_1, D_2, D_3, K_1, K_2, K_3, Pe_1, Pe_2, Pe_3, Cr_1, Cr_2, Cr_3, v, Δx, Δt, θ and φ values as input parameters.

Solution of model implementation is carried out based on Eq. (20) in the following spreadsheet format:

F3 = (-F2-$B$23*$B$18*(E2+G2-2*F2)/$B$2+$B$23*$B$14*($B$22*G2-$B$24*E2+$B$24*F2-$B$22*F2)/$B$2+$B$9*F2*$B$13-$B$25*E3-$B$31*G3)/$B$28 (22)

where F3, which is an intersection of the six column (F) and third row (3), represents the concentration in cell. Related terms are used in solving Eq. (20) has been shown in Eq. (22) as a spreadsheet format.

Before starting the simulation, firstly it is necessary to enter the initial and boundary condition values. After that, Eq. (22) is written to the F3 cell. After the completion of this process, the formulas in the F3 cells are copied and pasted to the relevant cell with the help of a basic macro and the iterative calculation is started. The sequence of calculation is then repeated for the second and subsequent iterations, until the termεis less than the error criterion at all nodes or the time index reaches the N value.

3. RESULTS AND DISCUSSION

3.1 Numerical applications

Take a continuous source in homogeneous isotropic groundwater system for example. Specific parameters are as follows (Clement et al, 1998).

The values of the various parameters used are $[NH_4]$ =0.42, $[NO_2]$ =0, $[NO_3]$ =0, R_{NH4}=1.6306, R_{NO2}=1.0352, R_{NO3}=1.0352, D_{L1}=221.9256, D_{L2}=120.7776, D_{L3}= 120.7776, v = 5.28 m/s, K_1= 0.0874, K_2=0.484, K_3=0.002. The space step and time step are taken to be Δx = 25 m and Δt = 1 s, respectively.

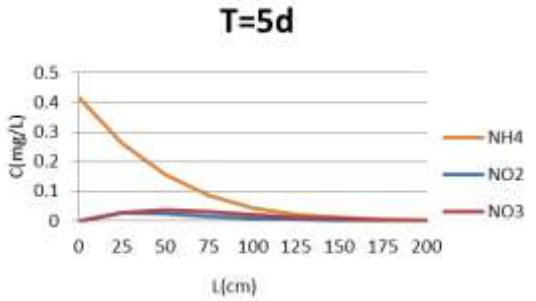

Fig2. Changing curve of concentration (T=5d)

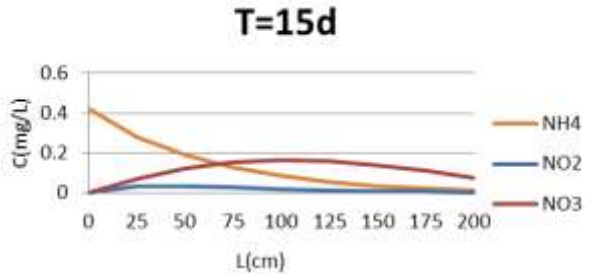

Fig3. Changing curve of concentration (T=15d)

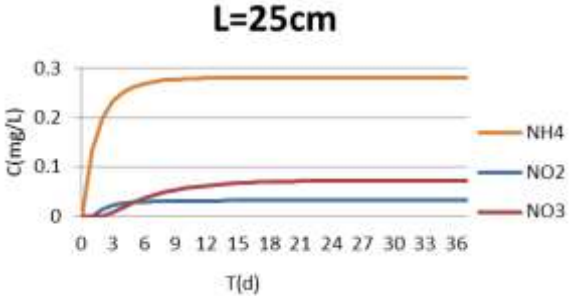

Fig4. Changing curve of concentration (L=25cm)

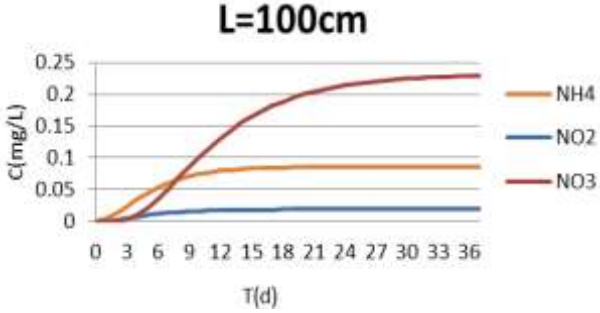

Fig5. Changing curve of concentration (L=100cm)

The analytical solution to the one-dimensional transport and transformation mathematical model of three nitrogen is given as

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$$C(x,t) = \frac{C_0}{2}\exp\left(\frac{vx}{2D}\right)\left\{\exp\left[-\frac{x}{2\frac{D}{R}}\sqrt{\left(\frac{v}{R}\right)^2+4K\frac{D}{R}}\right]\operatorname{erfc}\left[\frac{x-\sqrt{\left(\frac{v}{R}\right)^2+4K\frac{D}{R}}t}{2\sqrt{\frac{D}{R}t}}\right]+\exp\left[\frac{x}{2\frac{D}{R}}\sqrt{\left(\frac{v}{R}\right)^2+4K\frac{D}{R}}\right]\operatorname{erfc}\left[\frac{x+\sqrt{\left(\frac{v}{R}\right)^2+4K\frac{D}{R}}t}{2\sqrt{\frac{D}{R}t}}\right]\right\} \quad (23)$$

From Fig.6, BTCS model gives very close results to the analytical solution. Therefore, the model can be used to simulate three nitrogen transport and transformation problem.

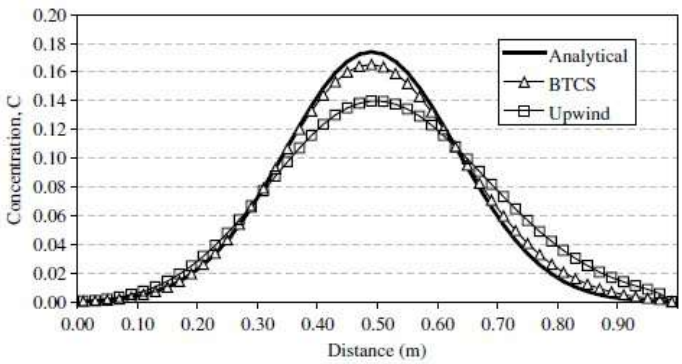

Fig 6. Comparison of analytical and numerical solution (BTCS scheme)

4. CONCLUSION

In this study, a mathematical model was developed to describe transformations and transport of nitrogen compounds in a saturated groundwater aquifer. From the Comparison of analytical and numerical solution (BTCS scheme), the model is feasible and it can provide a convenient tool for simulating the transportation and transformation for nitrogen in groundwater. With the change of the input parameters, the change in the model results can easily be observed graphically. Thus, the effect of the model parameters on the model accuracy, stability can be seen visually. The model not only can simulate one-dimensional solute transport, but also can be applied to two-dimensional case.

5. ACKNOWLEDGEMENTS

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