Optimizing First-order Rate Coefficients for Soil Nitrate Transformation Processes Applying an Inverse Method

X. M. Zhu¹, J. C. Shi², Q. Zuo²*, L. C. Wang², and W. J. Zheng²

ABSTRACT

It is extremely challenging to measure first-order rate coefficients for soil nitrate transformation processes directly, either in the laboratory or in the field. In this study, an improved inverse method was proposed to optimize the first-order rate coefficients by considering the intermediate changing processes of the integrated functions. A numerical experiment was designed to test the accuracy of the method in optimizing the coefficients. Comparisons between the optimized and theoretical results indicated that all the relative errors were within 10%. Data collected from a field experiment were used to validate the optimization procedure and to demonstrate its applications in practice. Using the established model and the estimated values by the inverse method, the simulated source-sink term (SST) distributions of September 2-12, 2007, were in good agreement, with the root mean squared error (RMSE) between them being as low as 0.00021 mg cm⁻³ d⁻¹. Based on the established nitrate transformation model, the distributions of soil water content and nitrate concentration during September 2-12, 2007, were simulated, and compared well with the measured profiles, with the RMSE of 0.023 cm³ cm⁻³ and 0.017 mg cm⁻³, respectively. The improved inverse method should be useful for optimizing the first-order rate coefficients for nitrate transformation, establishing the nitrate transformation model, and simulating the nitrate transport in the soil-plant system.

Keywords: Numerical simulation, Root-nitrate-uptake, Soil nitrate kinetics, Soil nitrate transformation.

INTRODUCTION

Nitrogen (N), an essential and key nutrient for plant growth and productivity, is meanwhile recognized as a major contributor to environmental pollution through nitrate (NO₃⁻-N) leaching and gaseous N emission (Arrobas and Rodrigues, 2013). The growing concern about the environmental impact of N fertilizer has enhanced the desire to simulate the transport and transformation of N in soils more accurately. Various simulation models of N turnover in the soil-plant system, differing in representation of processes, numerical algorithms and complexity have been developed in a number of countries (Cabon et al., 1991; Keating et al., 2003; Garnier et al., 2003; Del Grosso et al., 2005; Hansen et al., 2012). Comparisons reveal that the main discrepancies between models are often attributed to inadequate descriptions of the simultaneous processes of N turnover and incomplete definitions of input parameters (Wu and McGechan, 1998; Dinesh and Richter, 2002).

The nitrate transformation involves several complicated processes in soils, such as immobilization, nitrification, denitrification,
and uptake by roots. First-order kinetics remains the most commonly used approach to quantify reaction rates for these processes (Ma and Shaffer, 2001). The corresponding rate coefficients are then modified for considering the effects of temperature, water content, pH, oxygen, and so on, depending on individual authors of various models. Theoretically, the rate coefficients should be similar under optimal conditions when the process is described as the first-order kinetics controlled by the same factors. However, the suggested rate coefficients vary from model to model. How to determine these rate coefficients accurately and effectively becomes one of the main obstacles in model applications (Ma and Shaffer, 2001). Since the rate coefficients are very difficult to measure directly, the trial-error method is often used to obtain coefficients related to these rates, which may not be optimized in a strict mathematical sense (Shaffer et al., 2001).

To solve similar problems, inverse methods have in recent years presented attractive alternatives. In order to establish the root-water-uptake (RWU) model, a few inverse methods were used to optimize RWU parameters by minimizing the residuals between simulated and measured soil water contents (Musters and Bouten, 2000). Zuo and Zhang (2002) developed an inverse method to estimate the average distributions of RWU rate. Shi et al. (2007) applied the method successfully to estimate the source-sink term (SST) in nitrate transport equation i.e. convection-dispersion equation (CDE), and optimize the root-nitrate-uptake (RNU) factor, one of the first-order rate coefficients. However, they neglected the other transformation processes such as ammonium nitrification, immobilization and denitrification through designing an ideal soil column experiment.

The objective of this study was to optimize the first-order rate coefficients related to nitrate transformations applying an improved inverse method. Thereupon, the SST model was established and the dynamics of soil nitrate was simulated. A numerical and a field experiment were designed to examine the feasibility of optimizing transformation rate coefficients and simulating soil nitrate transport in soil-plant systems using the inverse method.

**MATERIALS AND METHODS**

**Water Flow in Soils**

Successful simulation of NO$_3$-N dynamics depends on accurate description of soil water movement. One-dimensional vertical soil water flow with RWU is simulated using Richards’ Equation as follows (Wu et al., 1999):

\[
C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} - 1 \right) \right] - S(z, t)
\]

\[ (1) \]

\[ h(z,0) = h_0(z) \quad 0 \leq z \leq L \]

\[ (2) \]

\[ \left[ -K(h) \left( \frac{\partial h}{\partial z} - 1 \right) \right]_{z=0} = -E(t) \quad t > 0 \]

\[ (3) \]

\[ h(L,t) = h_L(t) \quad t > 0 \]

\[ (4) \]

Where, \( h \) is the soil matric potential (cm); \( C(h) \) is the soil water capacity (cm$^{-1}$); \( K(h) \) represents the soil hydraulic conductivity (cm d$^{-1}$); \( z \) is vertical coordinate originating from the soil surface and positive downward (cm); \( t \) is time (d); \( h_0(z) \) is the initial soil matric potential in the profile (cm); \( E(t) \) is the soil surface evaporation rate (cm d$^{-1}$); \( h_L(t) \) is the matric potential at \( L \) (the lower boundary) (cm); and \( S(z, t) \) is defined by Wu et al. (1999) as follows:
$S(z,t) = S(z_r,t) = \gamma(\theta) S_{\text{max}}(z_r,t) = \frac{T_p}{L_{\text{rad}}(z_r)}$

Where, $z_r (= z/L_r)$ is the normalized root depth ranging from 0 to 1; $S_{\text{max}}(z_r,t)$ is the maximal specific water extraction rate under the optimal soil water conditions (cm$^3$ cm$^{-3}$ d$^{-1}$); $\gamma(\theta)$ is a dimensionless reduction function related to the effect of water stress; $T_p$ represents the potential transpiration rate (cm d$^{-1}$); $L_{\text{rad}}(z_r)$ is the normalized root length density distribution; and $\theta$ is the soil water content (cm$^3$ cm$^{-3}$).

**Nitrate Transport in Soils**

One-dimensional vertical movement of nitrate in the unsaturated zone is characterized by the CDE combined with a SST (Lafolie, 1991):

$$\frac{\partial \theta C_N}{\partial t} = \frac{\partial}{\partial z} \left[ \theta D(\theta, v) \frac{\partial C_N}{\partial z} - q C_N \right] + SST_N(z,t)$$

$C_N(z,0) = C_{N0}(z) \quad 0 \leq z \leq L$

$$\left[ - \theta D(\theta, v) \frac{\partial C_N}{\partial z} + q C_N \right]_{z=0} = Q_s(t) \quad t > 0$$

$C_N(L,t) = C_{NL}(t) \quad t > 0$

Where, $C_N$ is the concentration of NO$_3$-N, expressed as mass of NO$_3$-N per volume of soil solution (mg cm$^{-3}$); $q$ is the Darcy's flux (cm d$^{-1}$), $v = v \theta$, in which $v$ is the pore water velocity (cm d$^{-1}$); $C_{N0}(z)$ is the initial NO$_3$-N concentration distribution (mg cm$^{-3}$); $Q_s(t)$ represents the flux of NO$_3$-N at soil surface (mg cm$^2$ d$^{-1}$); $C_{NL}(t)$ is the NO$_3$-N concentration at the lower boundary (mg cm$^{-3}$); $SST_N(z,t)$ is the SST integrating the transformation processes of NO$_3$-N in soils (mg cm$^3$ d$^{-1}$); $D(\theta, v)$ is the hydrodynamic dispersion coefficient (cm$^2$ d$^{-1}$):

$$D(\theta, v) = \lambda \left| v \right| + \frac{\theta^3}{\theta^3} D_0$$

Where, $D_0$ is the diffusion coefficient for NO$_3$-N in pure water (cm$^2$ d$^{-1}$); and $\lambda$ represents the dispersivity (cm).

The $SST_N(z,t)$ unifies the transformation processes of NO$_3$-N in soils, expressed as follows (Bradshaw et al., 2013):

$$SST_N(z,t) = S_n(z,t) - S_m(z,t) - S_d(z,t) - S_u(z,t)$$

Where, $S_n(z,t)$, $S_m(z,t)$, $S_d(z,t)$, and $S_u(z,t)$, respectively, are the rates of ammonium nitrification, NO$_3$-N immobilization, denitrification, and root uptake per unit soil volume (mg cm$^{-3}$ d$^{-1}$), and defined by the following equations:

-Nitrification: ammonium $\rightarrow$ NO$_3$-N (Cabon et al., 1991):

$$S_n(z,t) = k_i \phi(T, \theta) C_0(z,t) \theta(z,t)$$

$\phi(T, \theta) = \begin{cases} 1.07 [\theta(z,t) - \theta_j(z)]/\theta_j(z) & \theta(z,t) \leq \theta_j(z) \\ 1.07 [\theta_j(z) - \theta(z,t)]/\theta_j(z) & \theta(z,t) > \theta_j(z) \end{cases}$
-Immobilization: NO$_3^-$-N $\rightarrow$ Organic matter (Cabon et al., 1991):

$$S_m(z,t) = k_2 \varphi_2(T', \theta) C_N(z,t) \theta(z,t)$$

$$\varphi_2(T', \theta) = \begin{cases} 
    k_2 1.05^{[-f(z,t)-T_m]} \frac{\theta(z,t)}{\theta_{j}(z)} & \text{if } \theta(z,t) \leq \theta_j(z) \\
    k_2 1.05^{[-f(z,t)-T_m]} \frac{\theta_j(z)}{\theta(z,t)} & \text{if } \theta(z,t) > \theta_j(z)
\end{cases}$$

-Denitrification: NO$_3^-$-N $\rightarrow$ N$_2$O (McGechan and Wu, 2001):

$$S_d(z,t) = k_3 \varphi_3(T', \theta) C_N(z,t) \theta(z,t)$$

$$\varphi_3(T', \theta) = \begin{cases} 
    0 & \text{if } \theta(z,t) \leq \theta_d(z,t) \\
    1.05^{[-f(z,t)-T_m]} \frac{\theta(z,t) - \theta_d(z,t)}{\theta_j(z) - \theta_d(z,t)} & \text{if } \theta_d(z,t) \leq \theta(z,t) \leq \theta_j(z)
\end{cases}$$

$$\theta_d(z,t) = 0.627 \theta_j(z) - 0.0267 \frac{\theta_j(z) - \theta(z,t)}{\theta_j(z)}$$

-RNU (Schoups and Hopmans, 2002):

$$S_j(z,t) = \delta S(z,t) C_N(z,t)$$

Where, $k_1$, $k_2$, $k_3$, and $\delta$, respectively, are the first-order rate coefficients for nitrification of ammonium, immobilization, denitrification, and root uptake of NO$_3^-$-N. $\delta$ is usually abbreviated as the dimensionless RNU factor ($\delta \geq 0$); $C_0(z,t)$ is the concentration of ammonium in the soil solution (mg cm$^{-3}$); $T'(z,t)$ is the soil temperature ($^\circ$C); $T_m$ is the optimum temperature ($^\circ$C) and chosen as $T_m = 35^\circ$C in this study (Cabon et al., 1991); $\theta_j(z)$ = the field water capacity (cm$^3$ cm$^{-3}$); and $\theta_d(z,t)$ is the threshold water content (cm$^3$ cm$^{-3}$).

Range of the First-order Rate Coefficients in the Literature

Retrieval results have shown that the immobilization coefficient, $k_2$, was neglected in many cases (Keating et al., 2003; McGechan and Hodda, 2010; Liu et al., 2011; Hansen et al., 2012), but occasionally used in very few models, with the value of around $0.02$ d$^{-1}$ (Cabon et al., 1991). It is generally accepted that the RNU factor $\delta$ may depend on the types of solute, plant species, and nutrient status of the plant. A value of $\delta \leq 1$ corresponds to a passive RNU, and $\delta > 1$ would correspond to active uptake (Schoups and Hopmans, 2002). The first-order rate coefficients for nitrification ($k_1$) and denitrification ($k_3$) changed greatly with location and model, but were generally within the range of $0.005$-$1.0$ and $0.00016$-$0.006$ d$^{-1}$, respectively.

Optimization Procedure for the First-order Rate Coefficients

The average $\overline{SST}_N(z_i,T)$ may be calculated as follows:

$$\overline{SST}_N(z_i,T) = \frac{1}{T} \int_0^T SST_N(z_i,t) dt = \frac{k_1}{T} \int_0^T f_1 dt - \frac{k_2}{T} \int_0^T f_2 dt - \frac{k_3}{T} \int_0^T f_3 dt - \frac{\delta}{T} \int_0^T C_N(z_i,t) S(z_i,t) dt$$

(16)
In order to minimize the errors brought about by the numerical integration, the following procedures were proposed to improve the method introduced by Shi et al. (2007).

1. Solve Equations (1)-(4) using the implicit finite difference method to obtain $h(z, t)$ and $\theta(z, t)$.

2. Estimate the average distribution of $SST_N(z, T)$ from 0 to $T$ using the inverse method (Shi et al., 2007).

3. Approximate $SST_N(z, t)$ in Equation (6) with the estimated $SST_N(z, T)$, and solve Equations (6)-(9) numerically for the distributions of $C_N(z, t)$ from 0 to $T$ using the implicit finite difference method.

4. Piecewise calculate the integrals of Equation (16) using the trapezoidal formula, on the basis of the continuous distributions of $\theta(z, t)$ and $C_N(z, t)$ from 0 to $T$, which were obtained by Step (1) and (3), respectively.

5. Optimize the coefficients $k_i$, $k_2$, $k_3$, and $\delta$ simultaneously based on Equation (16) using the linear multivariate least-squares procedure, with the retrieval range of the coefficients in the literature as the constraint conditions.

### Numerical Experiment

A numerical experiment was designed to test the accuracy and convergence of the method in optimizing the first-order rate coefficients for nitrate transformation processes as follows:

1. Input a set of data related to water flow and nitrate transformation in soils, which are listed in Table 1.

2. Solve Equations (1)-(4) using implicit finite difference method to obtain distributions of matric potential $h(z, t)$.

3. Solve Equations (6)-(9) using implicit finite difference method to obtain the theoretical distributions of soil nitrate concentration $C_N(z, t)$ at time $t = T$ on the basis of Equations (11)-(15) and the input data in step (1).

4. Choose some values $C_N(z_i,t)$ from $C_N(z, t)$ according to a specified spatial interval (SI) as the “measured” data points.

5. Fit the “measured” points $C^*_N(z_i,t)$ to a continuous and smooth nitrate concentration curve using the following algebraic polynomial (Huang, 2010):

### Table 1. Soil properties, RWU and nitrate transformation parameters, initial and boundary conditions in the numerical experiment.

<table>
<thead>
<tr>
<th>Parameters and data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil properties (Carsel and Parrish, 1988): $\theta_s = 0.450$ cm$^{-3}$ cm$^{-3}$, $\theta_i = 0.067$ cm$^{-3}$ cm$^{-3}$, $K_s = 10.8$ cm d$^{-1}$, $\alpha = 0.020$ cm$^{-1}$ and $n = 1.41$ in van Genuchten’s Equation (1980).</td>
<td></td>
</tr>
<tr>
<td>RWU parameters (Musters and Bouten, 2000): $L_r = 150$ cm, $r_p = 0.6$ cm d$^{-1}$.</td>
<td></td>
</tr>
<tr>
<td>Hydrodynamic dispersion (Valente et al., 2004): $D_0 = 1.64$ cm$^2$ d$^{-1}$, $\lambda = 0.3$ cm.</td>
<td></td>
</tr>
<tr>
<td>Nitrate transport and transformation parameters (Cabon et al., 1991; Lafolie, 1991; Schoup and Hopmans, 2002): $k_1 = 0.3$ d$^{-1}$, $k_2 = 0.02$ d$^{-1}$, $k_3 = 0.003$ d$^{-1}$, $\delta = 1.3$, $T = 25$ºC.</td>
<td></td>
</tr>
<tr>
<td>Ammonium concentration: $C_0(z, t) = 0.02$ mg cm$^{-3}$.</td>
<td></td>
</tr>
<tr>
<td>Initial soil water content distribution: $\theta (z, 0) = 0.3663+5.76(z-83.57)\times10^{-4}-2.0(z-83.57)^2\times10^{-6}$ (cm$^3$ cm$^{-3}$);</td>
<td></td>
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<tr>
<td>Upper boundary conditions: $E(t) = 0.03$ cm d$^{-1}$; $Q(t) = 0$.</td>
<td></td>
</tr>
<tr>
<td>Lower boundary conditions: $h(180, t) = -34.123$, then $L = 160$ cm, $h(L, t)$ was linearly interpolated; $C_N(L, t) = (0.334 - 0.00994t)/10$ mg cm$^{-3}$.</td>
<td></td>
</tr>
</tbody>
</table>
Table 2. Comparison of optimized first-order rate coefficients using M1 and M2.

<table>
<thead>
<tr>
<th>Range</th>
<th>$k_1$ (d$^{-1}$)</th>
<th>$k_3$ (d$^{-1}$)</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>0.005-1</td>
<td>0.00016-0.0006</td>
<td>$\geq0$</td>
</tr>
<tr>
<td>Optimized (M1)</td>
<td>0.045 (85%)$^a$</td>
<td>0.0002 (93%)</td>
<td>0.696 (46%)</td>
</tr>
<tr>
<td>Optimized (M2)</td>
<td>0.295 (1.7%)</td>
<td>0.0028 (6.7%)</td>
<td>1.278 (1.7%)</td>
</tr>
</tbody>
</table>

$^a$ The number in the parentheses represents the relative error between the theoretical values and the optimized results.
RESULTS AND DISCUSSION

Numerical Experiment

With the RWU and nitrate transformation parameters (Table 1), distributions of soil nitrate concentration at \( t = 10 \) d was simulated using implicit finite difference method. The “measured” nitrate concentrations for spatial interval \( SI = 5-10 \) cm (i.e. \( SI = 5 \) cm for \( 0 \leq z \leq 30 \) cm and \( SI = 10 \) cm for \( z > 30 \) cm) were generated according to Step (4) in Section on “MATERIALS AND METHODS—Numerical Experiment”, and then fitted using Equation (17).

Since the first-order rate coefficient for immobilization \( k_2 \) was just occasionally employed as 0.02 d\(^{-1}\) in very few cases, in this study, it was fixed as the retrieval value and not involved in the optimization process. The remaining coefficients i.e. \( k_1, k_3, \) and \( \delta \) were then optimized simultaneously using the method (M1) proposed by Shi et al. (2007) and the improved method (M2) in this study, respectively, and compared with the theoretical values in Table 2. The results showed that the relative errors between the theoretical and optimized coefficients using M1 were more than 40%, without an acceptable range. However, reliable optimization results were obtained by M2, with all the relative errors not more than 10%. Without considering the intermediate changing processes of the integrated functions, it would be almost impossible to get satisfactory and reliable optimization results using M1. In general, the improved method (M2) would be worth being recommended to optimize the first-order rate coefficients for soil nitrate transformation processes through applying the inverse method to estimate the SST of soil nitrate transport equation.

Field Experiment

Considering that the numerical experiment might not represent the practical situation, we discussed the applicability of the optimization procedure in further using the field experiment. The measured soil water content, nitrate and ammonium concentration distributions above the rooting depths on August 11, 21, September 2 and 12, 2007, are shown in Figures 1 and 2, respectively. Figure 2 indicated that the values of soil nitrate concentration near the
Figure 2. Distributions of: (a) Measured and simulated soil nitrate concentration; and (b) Measured soil ammonium concentration, from August 11 to September 12, 2007 in the field experiment. Horizontal bars are standard errors.

soil surface ($0 \leq z \leq 30$ cm) were relatively high, and decreased with increasing depth. However, soil ammonium concentration distribution did not show a regular tendency and its values showed relatively small changes in the whole profile, except for the depth from 20 to 50 cm on August 21, 2007.

Estimating RWU and SST

With the measured soil water content, nitrate, and ammonium concentration profiles, the average distributions of RWU rate and SST during the experimental period were estimated using the inverse method.
(Zuo and Zhang, 2002; Shi et al., 2007) as shown in Figures 3 and 4, respectively. The values of average SST during August 11-21 and September 2-12 in the upper area (about 0≤z ≤ 45 cm) was negative and became positive when z > 45 cm. The results indicated that the nitrate transformation in the upper parts of 0-45 cm was mainly by root uptake, immobilization, and denitrification, while in the depths below 45 cm, especially with the decrease of RNU rate, nitrification became predominated. The changing tendency of average SST was also consistent with the distributions of soil nitrate and ammonium concentration (Figure 2) and RWU rate (Figure 3).
Optimizing the First-order Rate Coefficients

To establish the nitrate transformation model, two measured soil nitrate profiles on August 11 and 21, 2007, were used to optimize the first-order rate coefficients for nitrate transformation processes through the improved method. Similar to that in the numerical experiment, the first-order rate coefficient for immobilization $k_2$ was also taken as 0.02 d$^{-1}$. The other coefficients for nitrate transformation were optimized as: $k_1 = 0.275$ d$^{-1}$, $k_3 = 0.0024$ d$^{-1}$, and $\delta = 1.53$. With the established soil nitrate transformation model, measured soil nitrate and ammonium concentration distribution, and other related information, the average distribution of SST during September 2-12, 2007, was simulated through Equations (6)-(9) using the implicit difference method. The simulated average SST profile agreed well with the estimated distribution using the inverse method (Figure 4), with the RMSE between them as low as 0.00021 mg cm$^{-3}$ d$^{-1}$. The result showed that the optimization procedure using the improved method would be reliable and effective to optimize the first-order rate coefficients and establish soil nitrate transformation model in the field.

Simulating Soil Water Flow and Nitrate Transport

Since the measured soil water content and nitrate concentration profiles during August 11-21, 2007, were used to establish the nitrate transformation model, only the dynamics of soil water and nitrate during September 2 to 12, 2007, were simulated. Equations (1)-(4), which describe the soil water flow in the soil-maize system, were solved using the implicit difference method. With the measured distributions of normalized root length density on September 2 and 12, 2007, and other information, soil water flow during September 2-12, 2007, was simulated. The simulated soil water content distribution on September 12, 2007, was comparable with the measured profile (Figure 1), with the RMSE of 0.023 cm$^3$ cm$^{-3}$ between them.

On the basis of soil water flow simulation, the established nitrate transformation model, Equations (6)-(9) were solved using the implicit finite difference method to simulate soil nitrate transport between September 2 and 12, 2007. The simulated distribution of soil nitrate concentration on September 12, 2007, was also shown and compared with the measured profile in Figure 2, which demonstrated that the simulated results and changing tendency matched the measured values well. The RMSE between the simulated and measured nitrate concentration distributions was 0.017 mg cm$^{-3}$. In the simulation, soil ammonium concentration between September 2 and 12, 2007, was linearly interpolated using the measured ammonium concentrations on September 2 and 12, 2007. The results showed that the linear interpolation of the ammonium concentration had little influence on the simulation, and the inverse method would be applicable to establish nitrate transformation model and simulate soil nitrate transport in the field.

It should be noted that the RNU factor $\delta$ used in this study only included the root uptake of nitrate, not considering the uptake of soil ammonium. Moreover, the information about the distribution of ammonium concentration had to be given as the measured values because the transport and transformation of soil ammonium were not incorporated, which would be inconvenient for the numerical simulation in practice. To understand the characteristics of N turnover in the soil-plant system well, it would be better to couple simulation of the nitrate and ammonium transport in soils simultaneously. However, many researchers have shown that the concentration of nitrate is often much higher than that of ammonium in dry land soils (Ju et al., 2004; Mohsenabadi et al., 2008). In this case, it would be reasonable to suppose that the root uptake of soil N could be predominated by RNU and the movement of ammonium could...
be ignored. Therefore, the optimization procedure proposed in this study would be useful for analyzing the RNU of the plant and the dynamics of nitrate in the soil-plant system.

The numerical and field experimental results showed that the inverse method could be a useful alternative to optimize the first-order rate coefficients for nitrate transformation processes, establish the transformation model, and simulate nitrate transport in soils. However, to understand the cycling of soil N in the soil-plant system completely, further attention should be paid to coupling simulation of soil nitrate and ammonium transformation and transport.

CONCLUSIONS

Due to the fact that the first-order rate coefficients for nitrate transformation processes are very difficult to measure directly, an improved inverse method was applied to optimize them. A numerical experiment and a field experiment were designed to test the accuracy and effectiveness of the method in optimizing these coefficients. The results showed that the inverse method could be a useful alternative to optimize the first-order rate coefficients for nitrate transformation processes, establish the transformation model, and simulate nitrate transport in soils. However, to understand the cycling of soil N in the soil-plant system completely, further attention should be paid to coupling simulation of soil nitrate and ammonium transformation and transport.

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بهینه سازی ضریب درجه اول نرخ فراپند دگرگونی نیترات خاک با کاربرد روش مکوس

چکیده

اندازه گیری مستقیم ضریب درجه اول نرخ فراپند دگرگونی نیترات خاک در آزمایشگاه و نیز در مزرعه چالشی برگرفته است. در پژوهش حاکم در روش مکوس اصلاح شده برای بهینه کردن ضریب درجه اول نرخ فراپند مزبور با در نظر گرفتن تغییرات فراپندیهای بیناینده در گروه فراپند دگرگونی پیشنهاد و استفاده شد. بنابراین، آزمونی عدیدی برای درست آزمایی روش مکوس در تغییر ضریب های بهینه طراحی شد. مقایسه نتایج بهینه شده و مقادیر نتیجه‌گیری (نرخ) نشان داد که همه خطاهای نسبی در محدوده 10% بود. نیز، داده‌های گردآوری شده از یک آزمون مزرعه‌ای برای اعتبار سنجی روش بهینه سازی و نشناد کاربرد آن در عمل استفاده شد. بر پایه مدل به دست آمده و ارقام برآورد شده در روش مکوس، توزیع عبارت مشخص کمتر (source-sink term) داده‌های پایه زمانی 2007-2012 توافق و هماهنگی خوبی داشتند و رشته میانگین مربعات خطا (RMSE) بین آنها به کمی 0.00021 mg cm^{-3} d^{-1} بود. بر پایه مدل به دست آمده برای دگرگونی نیترات، توزیع مقدار آب خاک و غلظت نیترات در پایه زمانی 2007-2012 شبیه‌سازی شد که نتایج با مقادیر اندازه‌گیری شده در نبرد خاک به خوبی مقایسه می‌شد و رشته‌های میانگین مربعات خطا ها به ترتیب به‌رابطه 0.023 بود. به این قرار، روش مکوس اصلاح شده برای بهینه سازی ضریب درجه اول نرخ دگرگونی نیترات خاک و ایجاد مدل دگرگونی نیترات و شبیه سازی انقلا نیترات در سامانه‌های خاک‌های مختلف می‌نماید.