Analysis of The Migration and Accumulation Process of Nitrate-nitrogen Pollutants in The Unsaturated Zone of Soil

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Abstract. In order to understand the migration process of nitrate-nitrogen pollutants in the shallow unsaturated zone of the soil, the Tianjin coastal dredger and typical fluvo-aquic soils in North China were used as the research objects. The Hydrus-1D software was used to establish a numerical model to simulate nitrate. The pollution process of nitrogen pollutants in the unsaturated zone of soil, the results show that: during the migration process of the two kinds of shallow vadose zones of soil, the nitrate-nitrogen pollutants migrate downward at the maximum concentration before reaching the maximum concentration. After the maximum concentration, the concentration of nitrate nitrogen in the soil no longer increases; due to the difference in the average particle size of the soil, the migration rate of nitrate nitrogen in fluvo-aquic soil is significantly greater than that in artificial dredger soil. Nitrate nitrogen is in the simulation period completely passing through the simulated soil layer, the fluvo-aquic soil is completely passed through by nitrate nitrogen at 2d, and the artificial dredge fill is completely passed through by nitrate nitrogen at 2.5d.

1 Introduction

The Scholars have conducted a large number of studies on the migration and accumulation of nitrogen pollutants in the soil. Weng Lingyun et al. [1] have conducted field experiments in Huangtuo Village, Qingyuan County, Hebei Province for a period of 6 years since 2010. In the continuous field experiment, the effects of different nitrogen application contents on the accumulation and leaching of soil nitrate nitrogen were studied; Zhang Xuexue et al. [2] studied the irrigation and silt soil under different irrigation water amounts and fertilization conditions based on the soil column simulation method, results show: the amount of nitrogen applied has the greatest impact on the cumulative effect of nitrate-nitrogen migration in the soil; Yang Ruxin [3] et al. used numerical simulation analysis to study the soil moisture-nitrate nitrogen dynamic transport law in different fertilization conditions and irrigation intensity scenarios. In recent years, numerical simulation analysis method has become one of the main methods to study the accumulation and change of nitrogen pollution in soil due to its advantages such as good economy, fast speed and good visualization effect [4].

In this study, Hydrus-1D was used to simulate and compare the one-dimensional vertical migration and accumulation process of nitrate-nitrogen pollutants in the typical artificial dredger fill soil in Tianjin coastal area and the typical fluvo-aquic soil in the unsaturated zone of the North China Plain, and analyze their accumulation characteristics and differences.

2 Model establishment

2.1 The basic equation

The basic equation of water movement does not consider the horizontal flow and lateral flow of water, but only considers the one-dimensional vertical migration process of water, the classic Richards equation is used to describe the basic migration process of water in Hydrus-1D, Richards equation is as follows:

$$\frac{\partial \theta}{\partial t}=\frac{\partial}{\partial z}\left[K\left(\frac{\partial h}{\partial z}+\cos\alpha\right)\right]-s \qquad (1)$$

$$k(h,z)=k_S(z)k_r(h,z) \qquad (2)$$

Where: θ is the soil volumetric water content cm^3/cm^3; t is the length of time for simulation; α is the angle between the direction of water flow and the vertical direction. In this paper, only the one-dimensional vertical movement of water is considered, so $\alpha=0$; Z is the soil depth cm; h is the pressure head of the soil (cm); s is the source-sink term (cm^3/cm^3t^{-1}); k_r is the relative hydraulic conductivity; k_S is the saturated hydraulic conductivity

2.2 Soil moisture transport equation

The soil moisture transport model is used to describe the process of moisture transport in the soil. Hydrus-1D provides six soil water transport models including single-porous media model, dual-porosity/dual-permeability media model, etc. The classic van Genuchten-Mualem model in the single-porous media model is used for water transport in the soil. The simulation prediction of the

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migration process does not consider the hysteresis effect of moisture.

The van Genuchten-Mualem equation is as follows：

$$\theta(h) = \begin{cases} \theta_\gamma + \frac{\theta_s - \theta_\gamma}{[1+|\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \qquad (3)$$

$$k(h) = k_s s_e^l \left[1 - (1 - s_e^{1/m})^m\right]^2 \qquad (4)$$

$$m = 1 - 1/n, \quad n > 1 \qquad (5)$$

Where: θ_s is the saturated soil moisture content; θ_γ is the residual soil moisture content; a, m, and n are the empirical parameters of the soil moisture characteristic curve; s_e is the effective soil moisture content; k_s is the saturated hydraulic conductivity; l is the soil pore connectivity parameters, usually take the average value 0.5

2.3 Solute transport equation

This study uses the convection-dispersion equation to describe the solute transport process, and does not consider adsorption and various reactions

$$\frac{\partial \theta c}{\partial t} + p\frac{\partial s}{\partial t} = \frac{\partial}{\partial x}\left(\theta D\frac{\partial c}{\partial x}\right) - \frac{\partial qc}{\partial x} - s \qquad (6)$$

In the formula: c is the liquid concentration of the solution, mg/cm^3; ρ is the soil bulk density; s is the solute solid phase concentration; D is the comprehensive dispersion coefficient; q is the volume flow flux density; S is the source-sink term.

2.4 Initial conditions and boundaries

This simulation process only considers the one-dimensional vertical transport of nitrate nitrogen in the soil, and does not consider its transformation process, so the upper boundary of the water flow model is set to a constant flux atmosphere Atmospheric Boundary Condition with Surface Layer, the lower boundary is set to Free Drainage; the upper boundary of the solute transport model is set to 10mg/L Constant Concentration Boundary Condition, and the lower boundary is set to Zero Concentration Gradient Boundary, the height of the simulated soil column model is 60cm, the initial pressure head at the top is set to 0cm, and the initial pressure head at the bottom is set to -60cm, uniformly distributed from the top to the bottom from 0 to 60cm.

2.5 Grid division and time step

During the simulation process, the 60cm simulated soil column was divided into 1cm equidistantly, and observation points were set at 20cm, 40cm, and 60cm soil depth to study nitrate nitrogen pollutants. Migration in the vertical direction; the total simulation time of this study is 4d, the initial time step is 0.01d, the minimum time step is 0.001d, and the maximum time step is 0.1d. This simulation process outputs a total of 6 time node data, respectively 0.5d, 1d, 1.5d, 2d, 2.5d, 4d to study the changes of nitrate nitrogen pollutants in the soil over time. The iteration information of this simulation process uses the default values of the Hydrus-1D model.

2.6 Determination of soil hydraulic parameters

The main parameters involved in this simulation process are soil hydraulic characteristic parameters, because the conversion process of nitrate nitrogen is not considered. The basic physical and chemical data of the coastal artificial dredger fill used in this simulation was obtained by Ge Feiyuan et al. and use the geotechnical test method. The percentage of sand (0.05~0.5mm) is 2.7%, and the percentage of powder (0.002~0.05mm) is the percentage is 83.3%, and the percentage of clay particles (0.0001~0.002mm) is 14% [5]; the basic data of the typical fluvo-aquic soil in North China is obtained through experiments by Guo Zifan et al., and the percentage of sand particles (0.05~0.5mm) is 26%, the percentage of powder particles (0.002~0.05mm) is 67.5%, and the percentage of clay particles (0.0001~0.002mm) is 6.5%[6]. Using the Neural network prediction function in the Hydrus-1D water flow module to calculate the soil hydraulic characteristic curve, input the proportion of sand, silt, and clay to obtain the required soil hydraulic characteristic curve parameters for the simulation（see Table 1）.

Table1. soil simulation parameter

Soil	θ_γ	θ_s	**α**	**n**	K_s	l
Dredger fill	0.0692	0.4774	0.0069	1.6245	17.06	0.5
fluvo-aquic	0.078	0.43	0.036	1.56	24.96	0.5

3 Simulation results and analysis

3.1 Vertical change of soil nitrate nitrogen

The concentration of nitrate nitrogen increases rapidly within 0-2.5d in the two soils at different depths, and becomes stable after reaching the maximum concentration. After 2.5d, the concentration no longer increases(see Figure 1, 2). That is, when the reclaimed water is used for agricultural irrigation, the nitrate-nitrogen pollutants in the reclaimed water migrate and accumulate in the soil is increased to the maximum value at different depths in the unsaturated zone. After the cumulative concentration of nitrate reaches the pollutant concentration, the concentration of nitrate nitrogen pollutants in the soil layer will not increase in the continuous irrigation time.

At the three observation depths(20cm,40cm,60cm), the concentration change trends of fluvo-aquic soil and artificial dredger fill are basically the same. At a depth of 20cm, the concentration of nitrate nitrogen changes from 0 to 99% of the solute concentration. The fluvo-aquic soil lasts 0.6964 days, and the artificial dredger fill lasts 1.1175d. At the depth of 40cm and 60cm, the fluvo-aquic soil also reached the maximum solute concentration significantly earlier than the artificial dredger fill soil. It shows that the migration rate of nitrate-nitrogen pollutants in fluvo-aquic soil is significantly greater than that of artificial dredger fill. The reason for this phenomenon may be due to the fact that the proportion of silt and clay particles in the artificial dredger fill soil is smaller than that of the fluvo-aquic soil. The soil particles are smaller and the gaps between soil particles are smaller, which has a stronger hindering effect on water flow and solute transport. This makes the migration rate of nitrate nitrogen in artificial dredger fill lower.

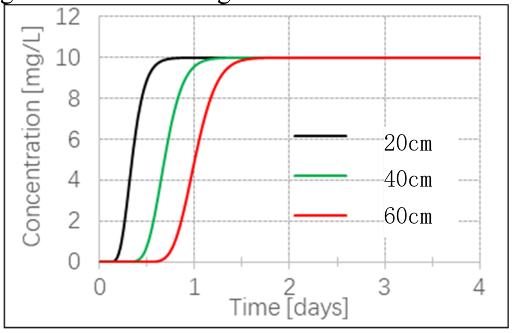

Figure 1. Variation curve of soil nitrate nitrogen concentration in fluvo-aquic soil

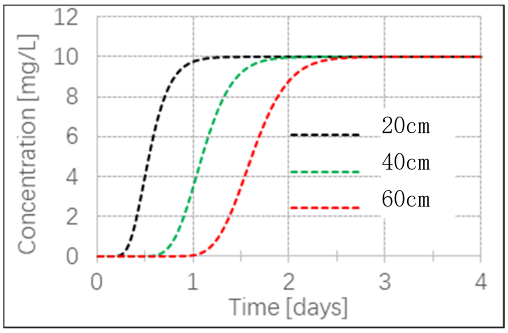

Figure 2. Variation curve of soil nitrate nitrogen concentration in artificial dredger fill soil

In order to further verify this point of view, the sandy loam soil is selected for simulation verification again,with larger average soil particles, and the sandy loam data is selected from the average sandy loam data that comes with the Water Flow Parameters module of the Hydrus-1D model(see Table 2).

Table2. soil simulation parameter

Soil	θ_r	θ_s	α	n	K_s	l
sandy loam	0.065	0.41	0.0075	1.89	106.1	0.5

At the three observation depths, the concentration change trends of sandy loam soil, dredger fill soil, and fluvo-aquic soil are basically the same. At a depth of 20 cm, the concentration of nitrate nitrogen changes from 0 to 99% of the solute concentration. The sandy loam soil lasts 0.1506 days, which is earlier than dredger fill soil and fluvo-aquic soil reach the maximum solute concentration. At the other two observation depths, sandy loam soil also reaches the maximum solute concentration significantly earlier than dredger fill soil and fluvo-aquic soil. The migration rate of nitrate-nitrogen pollutants in the unsaturated zone of soil is negatively correlated with the average soil particle size of the soil itself. This conclusion is more consistent with the research results of Wang Xiaodan et al. on the migration of the "three nitrogens" in the unsaturated zone of the Guanzhong Basin, Shaanxi[7]. .

If the appearance of nitrate nitrogen concentration in each soil layer is taken as the starting time, and the maximum concentration of nitrate nitrogen is reached as the ending time, then the time change of nitrate nitrogen pollutants from appearing and reaching the maximum concentration in each soil layer depth is obtained. The specific results are shown in the table3 and 4.

Table3. The time for the artificial dredger fill soil

Depth (cm)	20	40	60
Start time(d)	0	0.1519	0.353
maximum value time (d)	1.735	2.5627	3.2556
Last time(d)	1.735	2.4153	2.9026

Table4. The time for the fluvo-aquic soil

Depth (cm)	20	40	60
Start time(d)	0.2196	0.124	0.254
maximum value time (d)	1.0827	1.593	2.0207
Last time (d)	1.0608	1.469	1.7667

From Tables 3 and 4, it can be seen that the time step required for nitrate concentration to reach the maximum value in the soil layer will increase with depth, that is, the concentration migration rate slows down with the increase of depth, the reason is mainly due to the change of soil moisture at different depths.

3.2 Time series changes of soil nitrate-nitrogen concentration in the section of unsaturated zone

3.2.1 Analysis of concentration changes in artificial dredger fill soil

During the simulation process, the soil in the vadose zone of artificial dredging soil was completely penetrated by the nitrate nitrogen solution during the simulation period. In T2 time, the nitrate nitrogen had migrated to the bottom boundary, and the bottom boundary reached nitrate nitrogen pollution at T5 with the maximum concentration 10mg/L. Before T5, the nitrate nitrogen concentration in the soil gradually decreases from the top to the bottom of the vadose zone profile of the artificial dredging soil(see Figure 3). After T5, the nitrate nitrogen concentration in the entire vadose zone reaches the maximum value at 10mg/L.

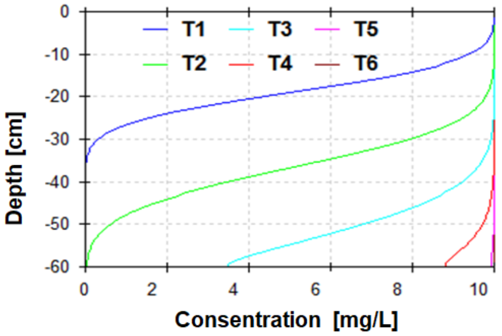

Figure 3. Variation curve of soil nitrate nitrogen concentration at different depths

(Note: T1, T2, T3, T4, T5, and T6 refer to 0.5d, 1.0d, 2.5d, 2.0d, 2.5d, 4d.)

3.2.2 Analysis of concentration changes of typical fluvo-aquic soil

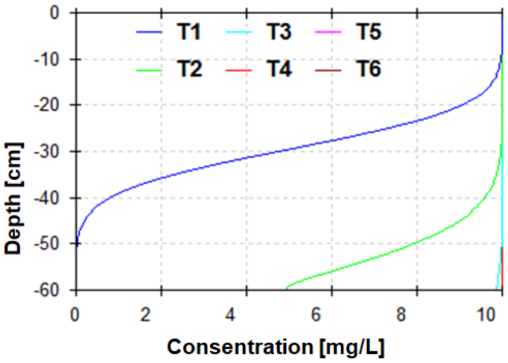

Figure 4. Variation of soil nitrate nitrogen concentration with depth

(Note: T1, T2, T3, T4, T5, T6 refer to 0.5d, 1.0d, 1.5d, 2.0d, 2.5d , 4d)

On the profile of the unsaturated zone in typical fluvo-aquic soil at different times, it can be seen from Figure 3 that during the simulation process, the soil in the typical fluvo-aquic zone of North China was completely penetrated by the nitrate nitrogen solution during the simulation period, and the bottom boundary was close to the maximum concentration value at T3, and reached the maximum concentration of nitrogen pollutants at T4 is 10 mg/L. Before T4, the nitrate nitrogen concentration in the typical fluvo-aquic soil zone profile from top to bottom in North China gradually decreases(see Figure 4). After T4, the nitrate nitrogen content in the entire unsaturated zone reached the maximum and stabilized at 10mg/L.

During T1 time, the migration depth of nitrate nitrogen in fluvo-aquic soil was significantly greater than that in artificial dredger fill; at time T2 and T3, nitrate nitrogen in both soils had migrated and diffused to the bottom boundary, but The cumulative concentration at the bottom boundary of the fluvo-aquic soil is significantly greater than the cumulative concentration at the bottom boundary of the dredger fill soil, indicating that the vertical migration rate of nitrate-nitrogen pollutants in typical fluvo-aquic soil is greater than that in artificial dredger fill soil.

4 Conclusion

During the migration process of nitrate-nitrogen pollutants in the vadose zone of artificial dredger fill soil, the migration and accumulation process in the soil at various depths will migrate and accumulate at the maximum concentration before the pollutant concentration is reached. After reaching the pollution source concentration, the nitrate nitrogen concentration in the soil does not continue to increase. That is, in the case of a longer scale, if the concentration of the nitrate nitrogen pollution source remains unchanged, the maximum concentration of the nitrate nitrogen pollutant concentration in the soil layer at each depth can eventually reach the pollution source concentration. Therefore, when the reclaimed water is used in the soil irrigation process, the nitrate nitrogen content must be strictly controlled, because the nitrate nitrogen concentration in the water will directly affect the nitrate nitrogen in the soil; the particle diameter of the soil itself will affect the nitrate nitrogen pollutants in the soil. The smaller the average soil particle diameter, the smaller the porosity between soil particles, the worse the transport of water and solute, and the slower the migration rate of nitrate-nitrogen pollutants in the soil; The migration rate in the soil is negatively related to the depth of the soil layer. The greater the depth of the soil layer, the slower the migration rate of nitrate nitrogen.

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