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Experiment and Numerical Simulation on Transportation of Ammonia Nitrogen in Saturated Soil Column with Steady Flow

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Abstract

Ammonium nitrogen in groundwater is one of the nutrient elements in the key monitoring indexes during the infiltration of water. Our objective of this study is to understand the adsorption and transportation characteristic of NH_3-N in the sandy loam. The calculated distribution coefficient (K_d) and retardation factor (R) of NH_3-N in the sandy loam was determined using the batch and Freundlich adsorption isotherm. We also got the break through curve (BTC) of NH_4^+ in saturated sandy loam by mixed displacement experiment. To verify the accuracy of the adsorption parameters, using the effluent data from a pulse change input miscible displacement experiments, by solving inverse problems of the equilibrium and chemical nonequilibrium convection-dispersion equation with the computer code (CXTFIT 2.0)， we estimated the optimized values of the retardation factor. These results indicate that the adsorption parameters calculated by our experimental data are in agreement with those estimated by the empirical formula.

Key words: ammonia nitrogen; convection-dispersion equation; retardation factor; numerical simulation

1. Introduction

Nitrogen fertilizer released during Human production and nitrogenous "three wastes"(waste gas, waste water and waste residues) from factories have seriously threatens the safe of Soil and underground water, which cause the attention on the transportation transition in soil aquifer. Ammonium-N is an inorganic pollutant with no direct toxic effects, when it reaches to a certain concentration or morphology occurred, it would change the environment or even a potential hazard to human health. High Nitrate level in drinking water in the baby body would produce too much blood protein disorder deformation. The action of nitrite and secondary amines would cause "Three-induce" nitrosamine of carcinogenesis, induced mutagenicity and teratogenesis. So it is imperative to control the input and release of Ammonium-N from the source. Nowadays, in the simulation of nitrogen transport in soil, deterministic models are widely used, among

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which convection–dispersion equation (short for CDE) [1] is the most widely applied. The application of Isotherm model and deterministic equilibrium model has achieved a large amount of result in researching pollutant transportation in soil, this dissertation takes use of this model in the condition of Ammonium-N transportation rules in soil under non-linear adsorption, in order to prevent further spread, predict and analyze its transportation range and degree in the soil to provide theoretical proof for the Ammonium-N transportation transformation numerical model of biochemical reaction.

2. Model theory

2.1. Freundlich isothermal adsorption model

Under a certain temperature conditions, There are two most commonly Isotherm model used in dilute solution: Freundlich Isotherm model and Langmuir Isotherm model. Many scholars have researched that the absorption of Ammonia nitrogen in the adsorbing medium abides with Freundlich Isotherm model. This dissertation calculates the liquidoid/solidoid distribution coefficient K_d and retardation factor based on Freundlich Isotherm model, which is:

$$G=KC_{eq}^{\ n} \quad (1)$$

G is the absorbance(mg/Kg)of the soil to NH_3-N in the equilibrium, K is absorption coefficient, n is constant of the Isotherm linearity. C_{eq} is the concentration(mg/L) of NH_3-N solution in the equilibrium.

The calculation equation [3] of retardation factor R is:

$$R = 1 + \rho K_d/\theta v \quad (2)$$

R is Retardation factor, ρ is dry soil dry bulk density, θv is soil volumetric water content(cm3/ cm3)

2.2. (Deterministic Equilibrium CDE)

Under stationary flow, the one-dimensional transform of absorptive solute can be got from Convection-Dispersion Equation(short for CDE) [4]:

$$\rho\frac{\partial s}{\partial t} + \theta\frac{\partial c}{\partial t} = \theta D\frac{\partial^2 c}{\partial x^2} - J_w\frac{\partial c}{\partial x} \quad (3)$$

3. Experiment methods

3.1. Experimental materials and equipment

Experimental material: sample soil is extracted from the loose sediments of the Yangtze floodplain, pH is 7.76, and Organic carbon is 0.33%. Measure soil particles by the Determination of forest soil particle-size analysis (mechanical analysis) (GB 7845-87).

Experiment equipment: HACH(DR2400)Portable Spectrophotometer, HACH(SensIon156)Portable multi-parameter instrument, chromatography of ions(DX-120), biserial thermostat water bath with 6 holes(Ronghua HH-6)，digital water bath oscillator(Ronghua SHA-B (A)).

Measure dried experimental soil 10.0g in 250mL conical beaker, input 100mL Ammonia nitrogen standard solution. In the experiment, the concentrations of initial NH_3-N standard solute (NH_4Cl，short for N) are 5mg/L，10mg/L，15mg/L，25mg/L，30mg/ L. Plug the conical beaker with prepared suspension (rotate speed is 200r/min), upward oscillation for 24 then the adsorption reaction reaches equilibrium status, after the reaction put suspension in to centrifugal machine for 10min(3000r/min), extract a certain amount of supernatant fluid to measure Ammonia-N content by Nessler reagent. Set parallel experiments based on various concentrations, and then set blank experiment with no soil; it is found that the absorption of vessel to Ammonia nitrogen can be ignored.

3.2. Saturated earth column miscible displacement experiment

The earth volume of zone of aeration in the experiment is made of synthetic glass with diameter of 14cm and 100cm of height, within it is 90cm homogenized sandy loam. After transferring sample soil into the lab, natural withering, removing impurities and sieving, then fill earth volume by controlling the Method of Bulk Density, set fixed density is 1.5g/cm3, initial water content is 9.9%， fill wet soil for every 5cm and tamp. Soil porosity is 43.4%. Control water with mariotte bottle, exhaust air and fill water by layers from top to bottom, infuse distilled water from column top with mariotte bottle, leaching the earth volume from top to bottom. After the earth volume is saturated , the volume of water in and out is 400mL/h， which means the water intake and discharge speed V is 6cm/h. Fill 100mL Ammonia nitrogen standard solute with concentration of 50mg/L instantaneously, replace Ammonia nitrogen solute to distilled water immediately after the earth volume is filled with Ammonia nitrogen solute, until the discharge Ammonia nitrogen concentration is close to earth volume background concentration. During the experiment process, extract sample water at the 15cm from the top, measure Ammonia nitrogen content in the water and record the time.

4. The calculation of retardation factor

It is very important to get the absorption parameters if soil to Ammonia nitrogen transportation time delay and retardation factor R. there are two means to get R : ① get retardation factor in the lab: calculate the factor with adsorption coefficient K_d of adsorption isotherm with batch equilibrium method; ② estimate retardation factor through convention- Diffusion Equation

4.1. Batch equilibrium experiment and the calculation of retardation factor R

From batch equilibrium experiment we can see that under 25℃, the absorption of sandy loam to Ammonia nitrogen in 5mg/L，10mg/L，15mg/L，25mg/L，30mg/L abides with Freundlich Isotherm model(equation 1). Use least squares technique to calculate parameters in the model, the results are shown in table 1. R is related coefficient; K, n is empirical constant; S is standard deviation.

Table 1 Freundlich isotherm model fitting equation in 25℃

experimental temperature	Freundlich equation lgG= nlgC + lgK	K	n	r	S
25℃	lgG=0.7042lgC +1.0472	11.148	0.7042	0.990	7.396

4.2. CDE model fitting of Ammonia - N data transportation in earth column

Take use of the CXTFIT 2 program code in Version 2.2 of STANMOD, which is developed by U.S. Salinity Laboratory, according to the BTC measured through miscible replacement experiment to solve the inverse problem of Convection-Dispersion Equation mathematical model, and then adopt non-linear least square optimization method to estimate retardation factor. Under stable one-dimensional conditions, fitting theoretical transformation model with experiment actual result to determine solute concentration distribution in different time and soil depth during the transportation process.

Within this research, first get the initial R value as 31.04 through batch equilibrium experiment, then substitutes it into equilibrium transportation model, set intake concentration as 50mg/L, time as 0. 25h and calculate BTC, the goodness of fitting is up to 96.4%. Estimate retardation factor R as 40.00, V 'is 5.6cm / h, D' is 0.3958 cm2 /h with the reverse problem of Convection-Dispersion Equation

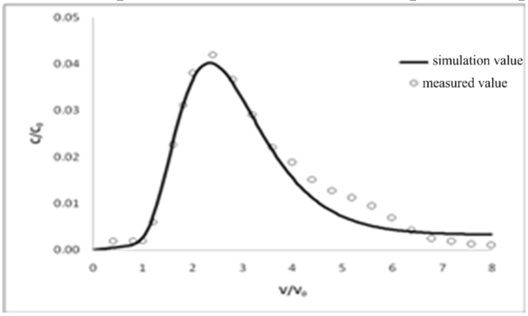

Fig 1 BTC measured value and simulation value of Ammonia - N in 15cm saturate sandy loam

5. Ammonia - N transportation simulating prediction of applying equilibrium CDE model under different boundary conditions

The transportation parameters got from the fitting of application model simulate the transportation rules of Ammonia nitrogen in saturate sandy loam under different boundary conditions; take "resurgent water soil aquifer processing system" as prerequisite to predict the transportation of Ammonia nitrogen in saturate sandy loam in different concentration, duration and infiltration speed. Based on the simulation data and take reference to the standard Ⅲ of the Quality standard for ground water(GB14848-93), set intake Ammonia nitrogen threshold value to ensure resurgent water reinjection, when the quality of underground water reaches standard Ⅲ, it means Ammonia nitrogen(record as N) ≤0.16 mg/L.

5.1. Different concentrations of influent ammonium

seasonal variations cause the changes of water concentration, based on Ammonia nitrogen first level A Standard of Discharge standard of pollutants for municipal wastewater (GB18918-2002), set summer (>12℃) intake Ammonia nitrogen concentration as C1=5mg/L and winter(≤12℃)intake Ammonia nitrogen concentration as C2=8mg/L. Simulate outlet water concentration variation law of earth volume in different concentrations within the same time (t1=1h，t2=2h)(see figure 2). The longer the continuous Ammonia nitrogen solute input, the higher the peak value, the later of peak time, the higher the residual concentration, and the greater risk to underground water.

5.2. Influent ammonium at different times

Soil has natural purification for pollutant, with the leaching by atmospheric precipitation, soil pollution can be repaired. Different accumulation of Ammonia nitrogen has various levels of pollution. The longer the intake time, the more the amount, the longer the natural purification time, the higher the pollution risk, if the intake concentration is C=5mg/L, then the intake time is t1=1h，t2=2h. with the simulation of CDE model and only considering the absorption effect, instantaneous intake Ammonia nitrogen content is

5mg/L resurgent water to simulate the time transportation rule(see figure 3) Ammonia nitrogen in sandy loam, and calculate the time of outlet Ammonia nitrogen reaching standard Ⅲ of underground water quality standard in the same depth(15cm). the simulation shows after Ammonia nitrogen reaches the Ⅲ standard with continuous 1h intake, 20.5h to approach the standard with continuous 2h intake. In the condition of stable intake water concentration, the more the continuous intake solute, the longer the time to decompose pollutant if only takes into consideration of the absorption of soul to Ammonia nitrogen and eluviations. In fact, under natural conditions, there is a large amount of microorganism in the soil, with enough carbon sources, Ammonia nitrogen would be transformed into nitrogen, trite nitrogen or organonitrogen. So in practical circumstances, Ammonia nitrogen peak time is longer with low peak value, which is affected by nitrification of nitrobacteria.

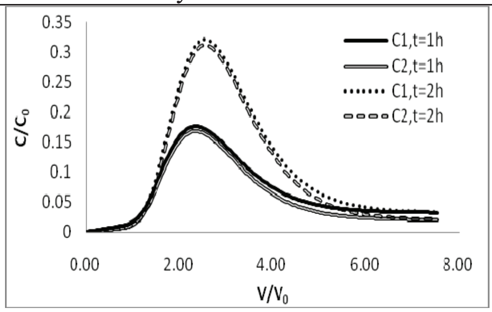

Fig 2 transportation simulation of different concentrations of Ammonia - N in saturated sandy loam

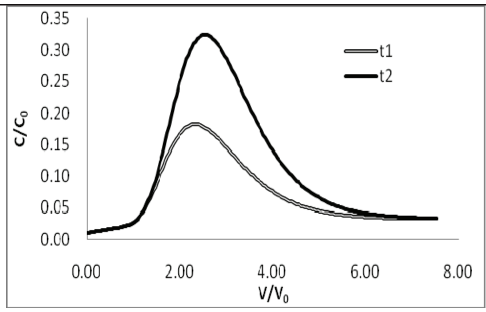

Fig 3 transportation simulation of 5mg/L Ammonia- N in saturated sandy loam at different times

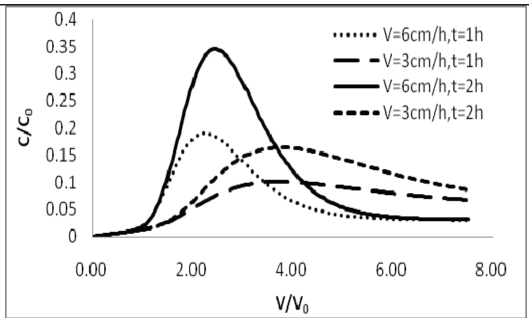

Fig 4 transportation simulation of 5mg/L Ammonia - N in saturated sandy loam before and after soil blockage

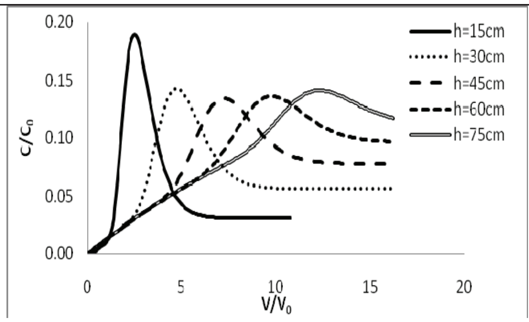

Fig 5 transportation simulation of 5mg/L Ammonia - N in different soil density

5.3. Ammonia - N transportation rules in different water rate

Soil aquifer system blockage causes the decrease of soil osmotic coefficient, which directly affects water intake speed; different water speed has a certain influence on Ammonia nitrogen transportation. Set osmose speed as V1=6cm/h， V2=3cm/h， V1>V2. Compare the influences of osmose speed to Ammonia nitrogen transportation under two reinjection C=5mg/L，t1=1h；C=5mg/L，t1=2h(see figure 4). Under the same concentration, compare the peaks of V1=6cm/h and V2=3cm/h, the frontal is sharp and narrow; peak value is high and comes very quickly. It means soil aquifer enhances the absorption of soil to Ammonia nitrogen because osmotic coefficient decreases and other factors, so that more Ammonia nitrogen are absorbed on soil particles. Under the same concentration but with different time and osmose speed, the length of duration affects the height of frontal, osmose speed influences frontal width and peak time.

5.4. motion rules of effluent ammonia nitrogen in different depth

Set soil thickness as h1=15cm，h2=30cm，h3=45cm，h4=60cm，h5=75cm, and simulate the transportation rule (see figure 5) of Ammonia nitrogen in various vertical heights. The deeper the soil, the later the peak time and the wider the duration, the value of peak tends to stable value along with the thickening of soil. So the thinner the soil layer, the greater the risk of contamination. The Ammonia nitrogen content at 75cm is the minimum, which means soil thickness determines the reaction time of physical, chemical or biological changes in soil aquifer, the thicker the soil depth, the longer the reaction time, the better the pollutant decomposition.

6. Conclusions

1, It is reasonable to describe the longitudinal transportation of Ammonia nitrogen in saturate stationary flow with Deterministic equilibrium CDE model

2,The longer of filling Ammonia nitrogen solute, the higher of peak value, the later of peak time, the higher of residual concentration, which brings more pollution threat to underground water .

3, The model only takes into account of adsorption and leaching, while there are a large amount of microorganism in natural soil, if there is enough carbon source, the activity of microorganism would affect the peak time and peak value of Ammonia nitrogen in soil.

4, From numerical simulation we can get, the decrease of soil osmotic coefficient in soil aquifer and water inlet speed strengthen the sorption of soil to Ammonia nitrogen, which means more Ammonia nitrogen is absorbed into soil particles.

5, Soil thickness determines the reaction time various kinds of physics, chemistry, biology in soil aquifer, the longer the reaction time, the better for pollutant decomposition

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