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Integrated numerical model of nitrogen transportation, absorption and transformation by two-dimension in soil-crop system

WANG Hong-qi*, SHU Yan, QI Yong-qiang, ZHANG Jun

(College of Water Sciences, State Key Joint Laboratory of Environmental Simulation and Pollution Control, Beijing Normal University, Beijing 100875, China. E-mail: whongqi@public.bta.net.cn)

Abstract: A series of simulation experiments of nitrogen transportation, absorption and transformation were conducted, and the different cropping patterns of winter wheat and wastewater irrigation plans were taken into consideration. Based on the experiments, an integrated model of crop growth, roots distribution, water and nitrogen absorption by roots, water and nitrogen movement and transformation in soil-crop system by two-dimension was developed. Parameters and boundary conditions were identified and an effective computing method for optimizing watering and wastewater irrigating plans was provided.

Keywords: nitrogen absorption and movement; integrated numerical model; soil-crop system

Introduction

Nitrogen is indispensable for the growth of crops. However, the contamination of nitrogenous compounds in water resources is becoming an increasingly serious problem, especially in intensive farming areas, because nitrogenous compounds left in the field may pollute groundwater through leaching or entering surface water body along with the rainwater. Detailed knowledge about the movement and transformation of these pollutants is very useful for us to design fertilizing plan in a manner that will minimize the negative environmental impacts. Analytical tools that are needed to simulate and predict the migration and transformation of pollutants through soil-crop system.

Many researchers have studied and developed models about the nitrogen cycle and the leaching of nitrate (Starr, 1974; Nye, 1977; Barber, 1986; Groot, 1991; Wang, 1992; 2002; 2003; Krug, 2002; Proporato, 2003; D'Odorico, 2003). Also, Reginato *et al*. developed the Michaelis-Menten absorption model of free boundary for root growth in 1991 (Reginato, 1991). Mengel and Pilbeam (Mengel, 1992) studied nitrogen absorption by plants and nitrogen transportation and transformation processes. Wang and Li (Wang, 1997) made integrated simulation analysis of the performance and patterns of nitrogen in crop growth and in migration process in consideration of crop growth, absorption by root and water, solute circulation process in SPAC system. Wang (Wang, 1997) designed soil column tests in laboratory to investigate nitrogen transportation and transformation in soil. Doussan *et al*. (Doussan, 1998) presented a numerical model simulating water uptake by root systems. Matthews *et al*. (Mattews, 2000) developed a model named CRACK-NP to investigate the potential impacts of tillage on rates of nitrate leaching from structured soils. Granlund *et al*. (Granlund, 2000) used a mathematical simulation model as a management tool to estimate the changes in nitrate leaching resulting from changes in cultivation practices in Finnish agriculture.

Most previous studies, however, have covered only part of the nitrogen transport and transformation process in soil-crop systems. Although some previous studies had considered the whole process-crop growth, roots distribution, roots absorption of water and nitrogen, and the movement and transformation of nitrogen in soil, they were inclined to describe these aspects in separate models and resolve them respectively. Actually, all of the aspects are interrelated. The movement of nitrogen in soil will have impact on the crop growth and thus the roots distribution, and inversely, the roots distribution will influence the movement of nitrogen in soil.

In this study, we developed and applied an integrated numerical model which simulates the processes of nitrogen transportation, absorption, and transformation in soil-crop system. This model took the following aspects into consideration: the impact of roots absorption on the crop growth, the impact of crop growth on the roots distribution, the root absorption of water and nitrogen and its impact on the movement of nitrogen in soil. Our main purpose is to build an integrated numerical model on the basis of simulation experiments and take a more global approach in assessing and developing an understanding of the movement and transformation of pollutants in soil-crop system.

1 Materials and methods

1.1 Simulation experiment condition

The experiment was conducted in a greenhouse under artificial conditions, in which there was an aerodynamics-adjusting system with air venting and cooling function. It includes soil column experiments and sectional two-dimensional bin scale physical simulation experiments, under bare, covered, winter wheat cropped conditions respectively. The design and grouping of simulation experiments are listed in Table 1.

Table 1 Design and grouping of simulation experiments

Group	Container for experiment				Covering	Planting
	Shape	Height, cm	Basal area, cm^2	Number		density, plants/cm^2
Group A	Cuboid	95	80 × 30	4	Planting winter wheat	0.0208
Group B	Cuboid	95	80 × 30	4	Planting winter wheat	0.1042
Group C	Colum	100	$\frac{19}{4}\pi$	5	Planting winter wheat	0.1415
Group D	Colum	100	$\frac{19}{4}\pi$	2	Bare	0
Group E	Colum	100	$\frac{19}{4}\pi$	2	Surface covering	0

Notes: Group C, D, E are mainly for parameters identification; group A and B are used for the development of integrated simulation model

1.2 Experiment procedure

We planted vernalized winter wheat in the devices of Group A, B, C. The irrigation intensity was designed according to physiological property of the winter wheat to ensure that the normal growth of plants. Meanwhile, appropriate quantity of P and N was added into the tested soil

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Foundation item: The National Natural Science Foundation of China (No. 29777001); * Corresponding author to regulate the crop development process rationally. High nitrogen concentration wastewater was used in early stage and middle stage of crop growth, low concentration wastewater or clean water was used in other stage. The quantity of nitrogen contaminant were used in different stages is shown in Table 2.

Table 2 Nitrogen quantity used in wastewater land treatment at different stages (mg/cm²)

Group	Date															Total
	March 1	March 28	April 4	April 18	April 25	May 7	May 8	May 12	May 21	May 22	May 28	June 1	June 4	June 5	June 9	
Group A	1.271	0.009	0.007	—	0.009	0.005	0.489	0.004	0.004	0.003	0.004	—	0.007	0.003	—	1.815
Group B	1.271	0.009	0.007	—	0.009	0.010	0.977	0.007	0.007	0.006	0.007	—	0.010	0.004	—	2.324
Group C	1.271	0.009	0.004	0.003	0.013	0.008	3.317	0.008	0.010	0.009	0.009	0.009	0.009	0.004	0.004	4.687

2 The integrated mathematical model by two-dimension in soil-crop system

2.1 Assumptions and prerequisites

These models were developed under certain assumptions and prerequisites for the rationality and practicability of the model. The assumptions and prerequisites are listed below.

- The quantity of nitrogen which crops needed all comes from nitrate nitrogen because the concentration of ammonia nitrogen is low, and ammonia nitrogen can be absorbed by crops only through nitration.
- Crop mass was classified into two categories, i. e. structure and storage, in the crop model. Structure is crop texture and storage is base for crop growth and transformation, usually considered as hydrocarbon compound or as some special content like nitrogen component.
- The cation exchange capacity (CEC) in soil is constant, and the cation adsorption-exchange process is instantaneous equilibrium.
- The impacts of temperature on the movement of water and solutes can be neglected. That is to say we can neglect the impacts caused by fluctuation of temperature.
- There only exits the interactivity among the ions of ammonia nitrogen, nitrate nitrogen and organic nitrogen in the system, and the other ions are non-interfering.

2.2 Expression of each sub-model

(1—1)Crop growth model

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{\mathrm{d}W_G}{\mathrm{d}t} + \frac{\mathrm{d}W_S}{\mathrm{d}t} = F_G E_A W_G$$

$$\frac{\mathrm{d}W_G}{\mathrm{d}t} = R\frac{W_G W_S}{W_S + bW_G}$$

$$W_S = SN$$

$$SN = 0 \quad W = W_0 \quad W_G = W_{G0} \quad t = 0$$

(1—2)Root growth, density and distribution model

$$R_w = \frac{f}{f+1}W$$

$$Z_r = \frac{a_r Z_{\max}}{1 + b_r \exp(-c_r t/t_m)} \quad t \leqslant t_{\max}$$

$$l(x,z,t) =$$

$$\begin{cases} \begin{cases} f_R R_w \alpha \exp(-\beta_1(x^2)\beta_2(z-30)^2) \\ \qquad z < Z_r\ t < t_{\max} \\ 0 \\ \qquad z > Z_r\ t < t_{\max} \end{cases} \\ \begin{cases} f_R R_w \alpha \exp(-\beta_1(x^2)\beta_2(z-30)^2) \\ \quad \left(1 - \alpha_r\left(\frac{t - t_{\max}}{t_m - t_{\max}}\right)\right) \quad z < Z_{\max}\ t > t_{\max} \\ 0 \quad z > Z_{\max}\ t > t_{\max} \end{cases} \\ R_w = 0 \quad l(x,z,t) = l(x,z,0) \\ \qquad t = 0\ z > 0 \end{cases}$$

(2—1)Water absorption by roots model

$$S_w = \begin{cases} 0 & \theta \leqslant \theta_0 \\ S_{\max}(t) \times \left(\frac{\theta - \theta_0}{\theta_d - \theta_0}\right) \times l(x,z,t) & \theta_0 < \theta \leqslant \theta_d \\ S_{\max}(t) \times l(x,z,t) & \theta_d < \theta \leqslant \theta_s \\ 0 & \theta > \theta_s \end{cases}$$

$$S_w = 0 \qquad t = 0$$

(2—2)Nitrogen absorption by roots model

$$C_a = \frac{2\pi D_{sh}}{\ln R - \ln r_c} / \left(\frac{F_{\max}}{K_m} + \frac{2\pi D_{sh}}{\ln R - \ln r_c}\right) - Q_w$$

$$Q_c = \frac{C_a}{K_m + C_a}F_{\max}$$

$$S_c = \frac{C_a}{K_m + C_a}F_{\max} \times l(x,z,t)$$

$$S_c = 0 \qquad t = 0\ x \geqslant 0\ z \geqslant 0$$

$$SN = \iiint S_c \mathrm{d}x\mathrm{d}z\mathrm{d}t$$

(3—1) Water transportation and absorption in soil by two-dimension model

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left(D_x(\theta)\frac{\partial\theta}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_z(\theta)\frac{\partial\theta}{\partial z}\right) - \frac{\partial K(\theta)}{\partial z} - S_w(x,z,t)$$

$$\theta = \theta_0(x,z) \qquad t = 0;\ x,z \geqslant 0$$

$$-D(\theta)\frac{\partial\theta}{\partial z} + K(\theta) = R(t) - E \qquad z = 0\ x,t \geqslant 0$$

$$-D(\theta)\frac{\partial\theta}{\partial z} + K(\theta) = 0 \qquad z = Z_D \quad x,t \geqslant 0$$

$$-D(\theta)\frac{\partial\theta}{\partial x} = 0 \qquad x = X_L\ x = X_R \quad z,t \geqslant 0$$

(3—2)NH_4^+ transportation and transformation in soil by two-dimension model

$$\frac{\partial(\theta C_1)}{\partial t} + \rho\frac{\partial S_1}{\partial t} = \frac{\partial}{\partial x}\left(D_{shxx}\frac{\partial C_1}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_{shzz}\frac{\partial C_1}{\partial z}\right) - q_x\frac{\partial C_1}{\partial x} - q_z\frac{\partial C_1}{\partial z} - k_2(\theta C_1 + \rho S_1) + k_1\theta C_N\frac{18}{14}$$

$$\frac{\partial S_1}{\partial C_1} = \frac{b}{\sqrt{C_1}}(S_{1m} - S_1)$$

$$S_1 = 0 \qquad C_1 = 0$$

$$C_1 = C_{10}(x,z) \qquad t = 0\ x,z \geqslant 0$$

$$D_{shxx}\frac{\partial C_1}{\partial x} - q_x C_1 = 0 \qquad x = X_L\ x = X_R \quad t,z \geqslant 0$$

$$D_{shzz}\frac{\partial C_1}{\partial z} - q_z C_1 = 0 \qquad z = 0;\ z = z_D \quad x,t \geqslant 0$$

(3—3) NO_3^- absorption, transportation and transformation in soil by two-dimension model

$$\frac{\partial(\theta C_2)}{\partial t} = \frac{\partial}{\partial x}\left(D_{shxx}\frac{\partial C_2}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_{shzz}\frac{\partial C_2}{\partial z}\right) - q_x\frac{\partial C_2}{\partial x} - q_z\frac{\partial C_2}{\partial z} + k_2(\theta C_1 + \rho S_1)\frac{62}{18} - k_3\theta C_2 - S_C$$

$$C_2 = C_{20}(x,z) \qquad t = 0\ x,z \geqslant 0$$

$$D_{\text{shxx}}\frac{\partial C_2}{\partial x} - q_x C_2 = 0 \qquad x = X_L\ x = X_R, t, z \geqslant 0$$

$$D_{\text{shzz}}\frac{\partial C_2}{\partial z} - q_z C_2 = R(t)C_0 \qquad z = 0\ x,t \geqslant 0$$

$$D_{\text{shzz}}\frac{\partial C_2}{\partial z} - q_z C_2 = 0 \qquad z = Z_D \quad x,t \geqslant 0$$

Where: W is the dry weight of crop, g/cm^2; W_G is the structural dry weight of crop; W_S is the weight of nitrogen in the crop; F_G is area-weight ratio of the leaves, cm^2/g; E_A is net assimilatory coefficient, g/(cm^2 · d); SN is total absorption of nitrogen, g/cm^2; R and b are constants; R_W is the dry weight of roots, g/cm^2; f is root-cap ratio, g/g; Z_r is the depth of roots when time is t, cm; Z is the depth of roots, cm; $Z_{\max}$ is the maximum depth of roots, cm; $t_{\max}$ is the time when Z reaches $Z_{\max}$, d; t_m is the length of the growing season, d; $l(x,z,t)$ is the distribution function of roots' length, cm/cm^3; f_R is roots length-weight ratio, cm/g; α, β_1 and β_2 are empirical constants about the roots' distribution; a_r, b_r and c_r are empirical constants about the roots' extension; S_w is the quantity of water which is absorbed by roots at unit time and unit soil volume, cm^3/(d·cm^3); C_a is the concentration of NO_3^- where it is near root's surface, mg/L; r_c is the average radius of roots, cm. $F_{\max}$ is the maximum nitrogen absorption speed of the roots, g/(cm·d); Q_w is the pumping capacity of roots, cm^3/(cm·d); Q_c is nitrogen absorption capacity of roots, cm^3/(cm·d·cm^3); S_c is the absorption capacity of nitrogen, mg/(d·cm^3); K_m is Michaelis constant, mg/cm^3; $R(t)$ is irrigation intensity, cm/d; E is evaporation from soil surface, cm/d; Z_D is the depth at the bottom of soil column, cm; X_L and X_R are the coordinate at the left and right of base point in horizontal direction respectively, cm; C_1, C_2 and C_N represent concentration of NH_4^+, NO_3^-, organic nitrogen in soil respectively, mg/L; S_1 is NH_4^+ concentration in solid phase, mg/kg; S_{1m} is the maximum concentration of NH_4^+ in solid phase, mg/kg; $C_{10}(x,z)$, $C_{20}(x,z)$ are the initial concentration of NH_4^+ and NO_3^- in soil respectively, mg/L; k_1, k_2, k_3 are mineralization rate, nitrification rate and denitrification rate respectively, 1/d.

3 Results and discussion

3.1 Numerical computation with the integrated model

The hydraulic and chemical dynamic parameters in the integrated model were determined by observing data of experiment Group B during sprouting period (before $t = 20$ d). The parameters for crop growth model and root distribution model were obtained from experiment Group C. All parameters were calibrated with the experimental data in the early phase.

The integrated model includes many sub models, and it requires integrated iterated computation in order to accomplish this systemic study. Fig. 1 shows the solution procedure.

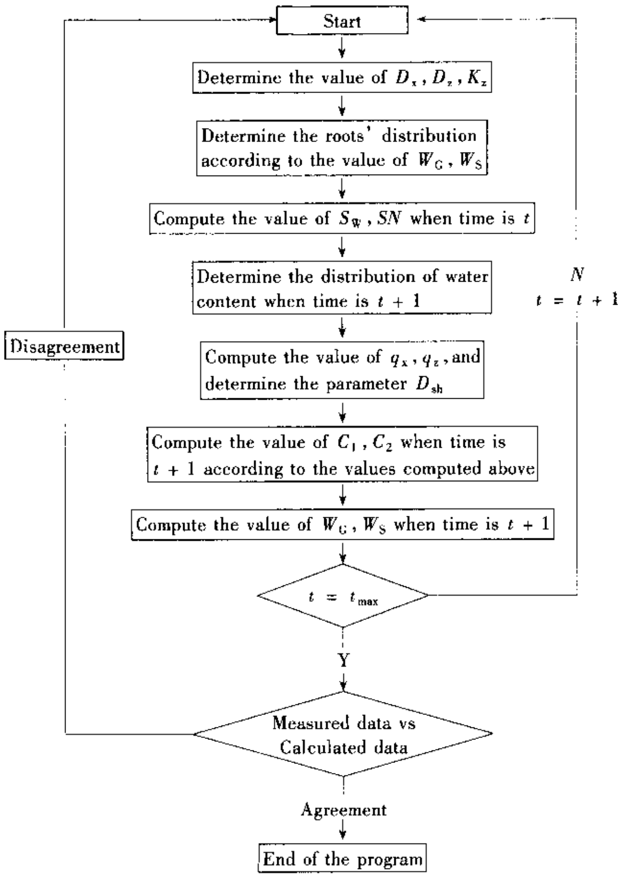

Fig. 1 Computation flow process chart of the integrated model

3.2 Simulation and analysis of winter wheat growth

Crop growth in Group A was simulated using crop growth model. The variation in different time and dynamic progress of crop dry weight (W), upper part weight of crop above the ground (W_P), crop structural dry weight (W_G), crop nitrogen weight (W_S) and crop growth factors were analyzed. Fig. 2 shows the dynamic progress of W and W_S, and we can find that both crop dry weight and crop nitrogen weight kept increasing during the experiment. In early phase of the experiment, crop dry weight (W) increased slowly, along with the increase of crop nitrogen weight (W_S), the accumulation of crop dry weight (W) was accelerated dramatically. Table 3 shows the increasing pattern of crop dry weight (W) in each growing phase in detail. Daily growth rate of crop in mature phase is three times that in tillering phase. That means accumulated nitrogen plays a significant role in crop growth, especially in mature phase under given environmental conditions.

Table 3 Statistical table of crop growth indices in each growing phase of Group A (Total amount in the whole device, 30 cm × 80 cm × 95 cm)

Crop period	Tillering phase	Jointing phase	Booting phase	Flowering phase	Filling phase	Mature phase
Date, month/day	4/19	4/30	5/6	5/21	6/12	6/20
Time, d	21	32	38	53	75	83
Weight of crop, g	10.88	22.90	30.23	67.96	157.70	173.46
Weight growth during each period, g	10.88	12.02	7.33	37.73	89.74	15.76
Days of each period, d	21	11	6	15	22	8
Rate of crop growth, g/d	0.52	1.09	1.22	2.52	4.08	1.97

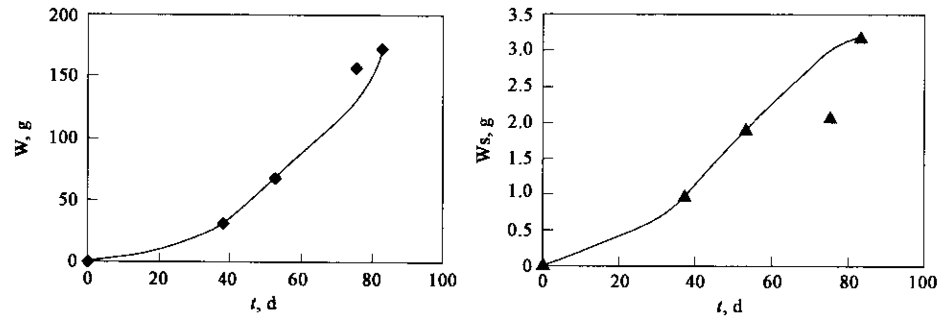

Fig.2 Dynamic process of crop dry weight(W) and crop nitrogen weight(W_S)
Total amount in the whole device, 30 cm × 80 cm × 95 cm;
—calculated value; ◆, ▲ measured value

3.3 Analysis of nitrogen absorption by roots

The dynamic processes of nitrogen absorption by roots in different layers and different horizontal distances are shown in Fig. 3. As shown in the profile, it is obvious that the intensity of nitrogen absorption in the surface layer is higher than that in deeper layer, and the deeper the roots are, the lower the intensity is. Also, nitrogen absorption intensity in the central is higher than that in the side and the more far from the central crop of the roots. Nitrogen absorption intensity and quantity are different in different growth phases. From filling stage to mature, nitrogen absorption intensity increases because of the increase of nitrogen demand. It is shown obviously in Fig.3 that nitrogen absorption intensity at the day 59 is higher than that at the day 19.

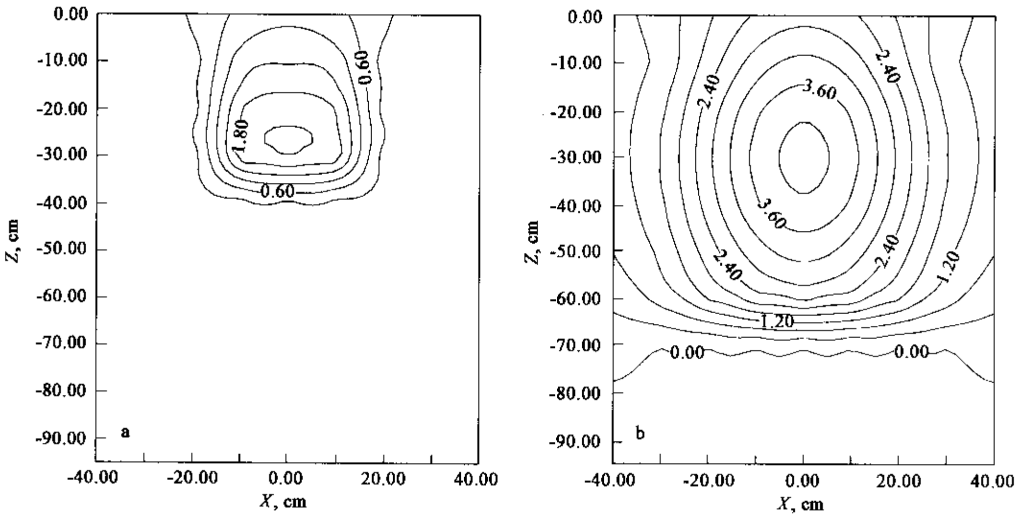

Fig.3 Profile of nitrogen absorption by roots at the day 19(a) and 59(b)

3.4 Simulation analysis of water and nitrogen movement, transformation and absorption in soil

In this integrated model, circulatory iteration method was used to integrate the whole process of crop growth, roots distribution, water and nitrogen absorption by roots, water and nitrogen movement, transformation and absorption, and crop growth, and a series of solutions were obtained. Restricted by the numerous factors which affect the processes mentioned above, water and nitrogen content in soil allocated and reallocated and thus formed different distributions of water and nitrogen content in profile. Fig.4 and Fig.5 show water and nitrogen content in the profile respectively. Affected by watering, water content in surface layer increases and this facilitates nitrogen to diffuse upward, thus nitrogen content in surface layer increases accordingly. On the other hand, the increases of water content also speeds up water absorption by roots. But the increase of nitrogen absorption is less than that of water absorption due to the influence of crop genetic factor, and the accumulation of nitrogen in surface layer of root which is carried by water facilitates the increase of nitrogen content at surface layer. From the analysis of nitrogen distribution in the sectional profile, a distinct high NO_3^- content zone exists in depth of 40—50 cm, and it keeps steadily high concentration from beginning of the experiment to the end. In horizontal direction, the change of water and nitrogen content is unconspicuous.

3.5 Comparison of measured data from experiment to calculated data and verification of model predictability

Based on the results of experiment Group A, analog computation of crop growth, water and nitrogen movement was performed. Then the observing data of experiment Group A was chosen to compare with the calculated data. The calculated crop dried weight and nitrogen content were compared with the measured data in Fig.2 and Table 4, Fig. 4 and Fig. 5 show comparison of measured and calculated data of water content in soil and nitrate nitrogen concentration in profile respectively. It is observed that measured data coincide with calculated data quite well, possessing strong ability of modeling reclamation.

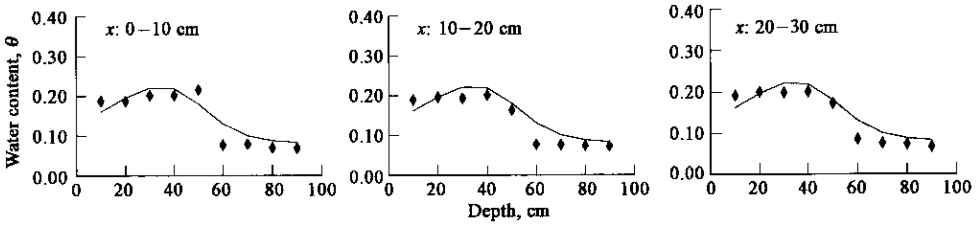

Fig.4 Water content in soil in profile at the day 44
—calculated ◆ measured

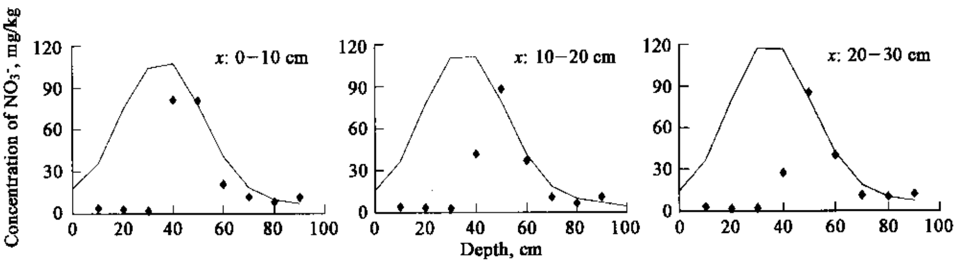

Fig.5 NO_3^- concentration in profile at the day 44
—calculated ◆ measured

Table 4 Statistics of crop growth power in each growth phase of Group A (Total quantity in 30 cm × 80 cm × 95 cm, g)

Time, d		38	53	75	83
Weight of crop(W), g	Measured	30.23	67.96	157.70	173.47
	Calculated	31.25	70.36	128.95	168.16
Weight of nitrogen in the crop (W_S), g	Measured	0.96	1.88	2.08	3.20
	Calculated	1.03	1.90	2.99	3.17

4 Conclusions

Based on the simulation experiments, which conducted under the conditions of different cropping patterns and different irrigation plants in the greenhouse, an integrated numerical model of crop growth, distribution of roots, water and nitrogen absorption by roots and transformation by two-dimension in soil-crop system was presented. In this model, the dynamic process of water, NO_3^-, NH_4^+ movement, absorption and transformation in two-dimension sectional profile in the soil-crop system was described.

From the coincidence of comparison, the accuracy of the model developed under the same condition was assured. Growth status of crops and roots, water and nitrogen absorption pattern by roots under different irrigation plans were simulated and analyzed due to the development and derivation of this integrated mathematical model. It is obvious that this model provides a primary computing method for selecting an efficient, productive irrigation and fertilizer application plan.

However, in this experiment, we used vernalization method rather than really put the wheat under winter conditions, and the experiment was conducted in greenhouse. These may cause the parameters in this model are not suitable for field experiment. Thus, if this model is used for field condition, corresponding adjustment should be made for the model to work correctly.

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