

LIANG Weili, LÜ Hongzhan, WANG Guiyan, D. J. Connor, G. M. Rimmington

# A simulation model-assisted study on water and nitrogen dynamics and their effects on crop performance in the wheat-maize system I: The model

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**Abstract** Based on data collected from field experiments, a comprehensive model was built on the *Ithink* (a registered trademark of iSee Systems) platform to simulate the dynamics of water and nitrogen, and crop performance in the winter wheat-summer maize double cropping system of the North China plain. The model, consisting of seven sub models, i.e. weather generator, phenology, biomass, dry matter partitioning, water balance, nitrogen balance, and nitrogen absorption and partitioning, well reflects water and nitrogen use and their relationship with crop yield under field conditions.

A vertical water movement equation is employed in the water balance sub model to account for movement between layers. Crop transpiration and soil evaporation are simulated separately according to potential evaporation, crop cover and a soil water deficit coefficient. Soil evaporation is from the surface layer only while crop transpiration comprises the total amount of water absorbed by the root system from all soil layers.

The model considers that nitrogen transformations, transfers and uptake are fulfilled by root systems. Transformation of nitrogen as mineralization, fixation and denitrification are responsive to soil moisture and temperature. Nitrogen movement is simulated with a convection-dispersion equation with nitrate as the soil solute. Nitrogen absorption and partitioning sub model includes the effects of water and nitrogen supply, crop nitrogen demand and nitrogen content in various crop organs. The model can be used to simulate crop yield,

water- and nitrogen-use efficiencies and water-nitrogen leaching to specific soil layers in different water and nitrogen management practices.

**Keywords** wheat, maize, cropping system, water, nitrogen, simulation, model

## 1 Introduction

It is estimated that the population in China will reach 1.6 billion in 2030 and by then the demand for cereals will increase by 180 million tons (Dai and Ye, 1999). In general, cereal production can be increased by expanding arable land area and/or increasing productivity. In China, the area of arable land is decreasing so the only option is to increase annual productivity over available arable land. Cultivar improvement, irrigation and fertilization remain the major means to increase productivity but the challenge now is also to develop applied practices to improve the efficiency of water and fertilizer use for the benefit of both environment and productivity.

The winter wheat-summer maize double cropping is the major cropping system for cereal production in the North China Plain that is already characterized by highly intensive crop production. The plain suffers the most severe water shortage in China while, at the same time, over irrigation and inefficient use of water are widespread. Depletion of ground water has been a big problem in the region with the result that a few depression cones of groundwater remain (Li, 1998). The current average annual nitrogen application is 192 kg/hm<sup>2</sup>, accounting for about one third of total national use. The large application of N, not uncommonly amounting to 500 kg/hm<sup>2</sup> (Ju, 2000), may pose an increasing threat through groundwater pollution by nitrate leaching. The result of a survey covering 14 counties in North China revealed that a serious nitrate pollution in groundwater with more than half of the 69 investigated sites exceeded the national standard 20 mg/L, while the highest was 300 mg/L (Zhang et al., 1995;

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LIANG Weili (✉), LÜ Hongzhan (✉), WANG Guiyan  
Department of Agronomy, Agricultural University of Hebei, Baoding  
071001, China  
E-mail: wayleel@hotmail.com; lvhongzhan@126.com.

D. J. Connor  
Faculty of Land and Food Resources, The University of Melbourne,  
Victoria 3010, Australia

G. M. Rimmington  
Office of Global Learning, Wichita State University, Wichita, KS 67206,  
USA

GB:5749-85, 1998). For a sustainable development, it is necessary to develop sustainable management practices to realize a high productivity together with high resource-use efficiency. This requires that people improve understanding of the effects of climatic factors and crop-water-nutrient management practices on availability and movement of water and nitrogen in the cropping system. Simulation modeling can serve as a powerful yet cheap tool to provide sound scientific data for the design of sustainable water and nitrogen management practices.

This paper presents a simulated model at the cropping system level for the natural conditions and management practices of the North China Plain. It operates on a daily time step including the major processes of water and nitrogen movement and transfer, as well as their interactions, and the simulation of the effects of water and nitrogen management practices on crop performance, nitrogen and water use, and their losses. Field data on crop performance and the dynamics of soil moisture and NO<sub>3</sub>-N content were collected at various soil layers together with crop data. The simulation software, *Ithink* (version 6.0) was used to construct the model as component sub models of crop production and of water and nitrogen dynamics. This study mainly discusses the detailed structure of the model and the testing calibration of the model together with a simulation study of the effects of water and nitrogen management practices on crop performance and environmental impact.

## 2 Weather data generator

This sub model provides daily weather data for the reference in related sub models.

Solar radiation is calculated with Brock's method (Brock, 1981; Cao and Luo, 2000). Solar radiation above the aerosphere is simulated as

$$\begin{aligned} \text{solext} = & 4.871 \times \frac{24}{\pi} \left( \frac{\text{daylength}}{2} \cdot \frac{2\pi}{24} \sin(\text{latitude}) \sin(\text{soldec}) \right. \\ & \left. + \sin \left( \frac{\text{daylength}}{2} \cdot \frac{2\pi}{24} \right) \cdot \cos(\text{latitude}) \cdot \cos(\text{soldec}) \right), \end{aligned} \quad (2.1)$$

$\text{daylength} =$

$$\begin{cases} 0.1333 \times 57.3 \times \text{Arc tan} \left( \sqrt{1 - \cosh^2} / \cosh \right) & \cosh \geq 0, \\ 0.1333 \times (180 + 57.3 \times \text{Arc tan} \left( \sqrt{1 - \cosh^2} / \cosh \right)) & \cosh < 0, \end{cases} \quad (2.2)$$

$$\cosh = \text{Tan}(\text{latitude} / 57.3) \cdot \text{Tan}(\text{soldec}), \quad (2.3)$$

$$\begin{aligned} \text{soldec} = & 23.4\pi / 180 \\ & \cdot \text{Cos}(2\pi(\text{Julian} \cdot 0.9863 + 0.9863 / 365)), \end{aligned} \quad (2.4)$$

where  $\text{latitude}$  stands for latitude at the field site,  $\text{daylength}$  for daylength at the field site,  $\text{soldec}$  for the latitude where the

sun is vertically overhead at solar noon,  $\cosh$  for cosine of sunshine angles at sunrise and sunset, and  $\text{Julian}$  for the day of the year starting as 1 on January 1, and  $\text{solext}$  for solar radiation above the aerosphere.

Solar radiation ( $\text{solrad}$ ) is calculated with the following equation:

$$\text{solrad} = \begin{cases} 0.75 \cdot \text{solext} & \text{clear,} \\ 0.25 \cdot \text{solext} & \text{cloudy.} \end{cases} \quad (2.5)$$

## 3 Phenology sub model

### 3.1 Wheat

Development stage is represented with five-stage numeric index, i.e. 0 for sowing, 1 for emergence, 2 for stem elongation, 3 for heading, and 4 for maturity.

For individual cultivars, crop growth is affected by environment, especially by day length and temperature. Thus, the basic model of wheat growth can be depicted as

$$dM/dt = e^k \cdot (TE)^p \cdot (PE)^q \cdot f(EC), \quad (3.1)$$

$$\begin{aligned} TE = & (Ti - Tbi) / (Toi - Tbi), \text{ when } Ti < Tbi \text{ then } Ti = Tbi \\ \text{or when } & Ti > Toi \text{ then } Ti = Toi, \end{aligned} \quad (3.2)$$

$$\begin{aligned} PE = & (PLi - PLbi) / (PLoi - PLbi), \text{ when } PLi < PLbi \text{ then} \\ PLi = & PLbi \text{ or when } PLi > PLoi \text{ then } PLi = PLoi, \end{aligned} \quad (3.3)$$

where  $dM/dt$  stands for the daily development rate of winter wheat,  $TE$  for the temperature factor, indicating the non-linear effect of temperature on wheat development,  $p$  for the temperature coefficient reflecting sensitivity of a cultivar to temperature at certain stage,  $PE$  for the coefficient of photoperiod effect,  $q$  for a genetic coefficient of photoperiod effect indicating sensitivity of a cultivar to photoperiod at certain stage,  $EC$  for a coefficient reflecting the effect of other factors such as depth of seed sowing,  $k$  for the basic development coefficient determined by cultivars: A high value indicates fast development and early maturity of the cultivar,  $Ti$  for the temperature at stage  $i$ ,  $Tbi$  for the minimum temperature for wheat growth at stage  $i$ ,  $Toi$  for the optimum temperature for wheat growth at stage  $i$  (possible damage that may occur when  $Toi < Tbi$  or  $Ti > Toi$  is not included because the problem does not occur in this area),  $PLi$  for the average daylength at stage  $i$ ,  $PLoi$  for the optimum daylength at stage  $i$ , and  $PLbi$  for the marginal daylength at stage  $i$ .

Calculations at different stages are as follows.

#### 3.1.1 Sowing to emergence

The delay of wheat emergence from sowing is related to temperature, seeding depth and soil moisture. In practice, soil moisture is an unlimited factor for emergence so growth rate

at this stage can be described as a function to temperature and seeding depth:

$$\begin{aligned} dM1/dt &= 1/D1 = f(D1) \times f(TE1) \times f(depth) \\ &= e^{k1} \times ((T1 - Tb1)/(To1 - Tb1))^{p1} \\ &\quad \times (1.5299 \times e^{(-0.0978 \times depth)}), \end{aligned} \quad (3.4)$$

where  $Tb1$  stands for the minimum temperature for wheat seed emergence (here 1°C),  $To1$  for the upper limit of optimum temperature for emergence (here 17.5°C),  $Depth$  for seeding depth (4 cm is adopted in this study),  $k1 = -1.891$ ,  $p1 = 1.19$ .

### 3.1.2 Emergence to stem elongation

It is assumed that the wheat crop responds first to vernalization, then to photoperiod, and that stem elongation indicates the completion of photoperiodic response (Wang, 1995).

#### (1) Vernalization

The coefficient  $Ve$  is used to represent daily progress of vernalization, shown as

$$Ve = \begin{cases} (VT - VTb)/(VT_{O1} - VTb) & VTb < VT \leq VT_{O1}, \\ 1.0 & VT_{O1} < VT \leq VT_{O2}, \\ (VTm - VT)/(VTm - VT_{O2}) & VT_{O2} < VT \leq VT_{O2}, \\ 0 & VT \leq VTb, VT \geq VTm, \end{cases} \quad (3.5)$$

where  $VTb$  stands for the minimum temperature of vernalization (here -4°C),  $VT_{O1}$  for the lower limit of optimum temperature for vernalization (here 3°C),  $VT_{O2}$  for the upper limit of the optimum temperature of vernalization (here 7°C), and  $VTm$  for the maximum temperature of vernalization (here 18°C).

It is assumed in this model that vernalization is accomplished when accumulated vernal days reach 40, thus

$$\frac{dM2}{dt} = \frac{1}{D2} = E^{K_{21}} (Ve)^{P_{21}}, \quad (3.6)$$

where  $K_{21} = -4.211$  and  $P_{21} = 0.606$ .

#### (2) Photoperiod

High temperature and long days can promote the photoperiodic response, shown as

$$\frac{dM_{22}}{dt} = \frac{1}{D_{22}} = E^{K_{22}} \cdot \left( \frac{T_{22} - TB_2}{TO_2 - TB_2} \right)^{P_{22}} \cdot \left( \frac{PL - PLB}{PLO - PLB} \right)^{Q_{22}}, \quad (3.7)$$

where  $K_{22} = -2.995$ ,  $Tb_2 = 20^\circ\text{C}$ ,  $PLB = 8$  h,  $PLO = 18$  h,  $P_{22} = 1.836$ , and  $Q_{22} = 0.294$ .

### 3.1.3 Stem elongation to heading

$$\frac{dM_3}{dt} = \frac{1}{D_3} = E^{K_3} \cdot \left( \frac{T_3 - TB_3}{TO_3 - TB_3} \right)^{P_3}, \quad (3.8)$$

where  $TB_3 = 3^\circ\text{C}$ ,  $TO_3 = 20^\circ\text{C}$ ,  $K_3 = -2.7$ , and  $P_3 = 1.386$ .

### 3.1.4 Heading to maturity

Temperature alone determines the duration of this stage of seed formation, shown as

$$\frac{dM_4}{dt} = \frac{1}{D_4} = E^{K_4} \cdot \left( \frac{T_4 - TB_4}{TO_4 - TB_4} \right)^{P_4}, \quad (3.9)$$

where  $TB_4 = 9$ ,  $TO_4 = 22$ ,  $K_4 = -3.416$ , and  $P_4 = 1.28$ .

### 3.2 Maize

The minimum temperature for maize growth is set at 10°C (Wang, 1995) and the development indices are defined as: 0—sowing; 1—emergence; 2—stem elongation; 3—tasseling; 4—maturity. The phenostage of maize ( $M_{pheno}$ ) is calculated with the following formula

$$M_{pheno} = \frac{\sum_{i=1}^n (Ti - 10)}{TUi}, \quad (3.10)$$

where  $Ti$  stands for average temperature at stage  $i$ , and  $TUi$  for degree days needed at stage  $i$ ; thus, the development rate of maize can be described as

$$\frac{dDi}{dt} = \frac{1}{Di} = \frac{Ti - 10}{TUi}. \quad (3.11)$$

The values of  $TUi$  adopted in this model are listed in Table 1.

**Table 1**  $TUi$  value at various stages for maize cultivar Ludan 14

Stage	Sowing-emergence	Emergence-stem elongation	Stem elongation-flowering	Flowering-maturity
$TUi$ value	80	447	441	528

## 4 Biomass production sub model

### 4.1 Wheat

#### 4.1.1 Photosynthesis

As described by Monsi-Saeki (Monsi et al., 1973; Carbon et al., 1991), the relation between photosynthetic rate of single leaf and its incident solar radiation can be represented with the following equation:

$$P = B \cdot P_{max} \cdot PAR / (B \cdot PAR + P_{max}), \quad (4.1)$$

where  $P$  stands for photosynthetic rate of single leaf, in  $\text{g CO}_2/\text{m}^2 \cdot \text{h}$ ,  $B$  for initial photosynthetic rate, i.e. the slope of response curve of radiation-photosynthetic rate (here  $1.4 \times 10^{-5} \text{g CO}_2/\text{J}$ ),  $PAR$  for photosynthetically active

radiation, assumed to be 50% of global radiation, and  $P_{\max}$  for the maximum photosynthetic rate at saturating radiation, which depends on cultivar, temperature, and water and nutrient supply.

The relation of  $P_{\max}$  to unit leaf area nitrogen content ( $SPLN$ ) is presented in Eq. (4.2) (Wang, 1995).

$$P_{\max} = 0.83 \times \left[ \frac{2}{1 + \text{EXP}(-1.45 \times (SPLN - 0.8))} \right] \times 3.6. \quad (4.2)$$

The optimum temperature range for photosynthesis of winter wheat is 15–20°C (Jiang and Liang, 1994), thus

$$P_T = \begin{cases} P_{\max} \cdot \sin(\pi Tave/35) & 0 < Tave < 35, \\ 0 & Tave \leq 0, Tave \geq 35. \end{cases} \quad (4.3)$$

Since  $P_{\max}$  is affected by water regime, the water deficit factor  $F_{wat}$  (Jiang and Liang, 1994) is used to modify it to specific water status ( $P_w$ ). Here  $F_{wat}$  is simplified as

$$P_w = P_{\max} \cdot F_{wat},$$

$$F_{wat} = \begin{cases} 0 & wt < w_1, \\ (w_t - w_1)/(w_2 - w_1) & w_1 \leq wt < w_2, \\ 1 & w_2 \leq wt \leq w_3, \\ 0.5 + 0.5(w_t - 1)/(w_3 - 1) & w_t > w_3, \end{cases} \quad (4.4)$$

where  $w_t$  stands for soil water content to the depth of 120 cm during crop growth,  $w_1$  for coefficient (at –15 bar) of soil water content in the depth of 0–120 cm,  $w_2$  for the lower limit of available soil water content during crop growth (here 60% of field capacity), and  $w_3$  for the upper limit of available soil water content during crop growth (here 85% of field capacity).

The photosynthetic rate of the wheat crop is then the dual integral of leaf photosynthetic rate over  $LAI$  and daylength,

$$W_{phos} = \int_0^{daylength} \int_0^{WLAI} B \cdot P_{\max} \cdot PAR / (B \cdot PAR + P_{\max}). \quad (4.5)$$

The intensity of solar radiation decreases from top to bottom of the crop canopy following Beer-Lambert's Law, so, the average intensity of solar radiation ( $I$ ) at a specific height in the crop canopy can be calculated as

$$I = I_0 \cdot E^{(-WK \cdot WLAI)}, \quad (4.6)$$

where  $I_0$  stands for solar radiation (solard) above the canopy,  $WK$  for light extinction coefficient of the canopy (here 0.7), and  $WLAI$  for leaf area index of wheat calculated in the biomass partitioning sub model.

Daily photosynthetic rate of the wheat canopy can be calculated by replacing  $PAR$  in Eq. (4.5) with Eq. (4.6). When unit of measurement is changed to g (CH<sub>2</sub>O)/m<sup>2</sup>·d, Eq. (4.5) can be rewritten as

$$W_{phos} = (0.682 \cdot daylength \cdot P_{\max}/0.7) \cdot \text{LOGN}((P_{\max} + 1.4 \cdot 10^{-5} \cdot 0.5 \cdot solrad \cdot 106/daylength)/(P_{\max} + 1.4 \cdot 10^{-5} \cdot 0.5 \cdot solrad \cdot 10^6 \cdot e^{(-0.7 \times WLAI)}/daylength)). \quad (4.7)$$

#### 4.1.2 Respiration

$$resp = rresp + sresp = \beta \cdot Q_{10}^{\left(\frac{T-25}{10}\right)} \cdot WTb + \alpha \cdot phos, \quad (4.8)$$

where  $resp$  stands for daily respiration of the wheat canopy,  $rresp$  for maintenance respiration,  $sresp$  for growth respiration,  $WTb$  for total biomass of the wheat crop,  $Q_{10}$  for respiratory quotient of wheat crop at the temperature of 25°C with a general value of 2,  $\alpha$  for respiratory coefficient (here 0.34), and  $\beta$  for maintenance respiratory coefficient (here 0.002 5 before and after grain filling).

#### 4.1.3 Biomass production

Daily biomass production ( $Npho$ ) is the daily photosynthetic gain minus the respiratory loss, i.e.,

$$Nphos = phos - (rresp + sresp). \quad (4.9)$$

### 4.2 Maize

#### 4.2.1 Photosynthesis

As in wheat model, maize photosynthetic rate is calculated as

$$M_{phos} = (0.682 \cdot daylength \cdot P_{\max}/MK) \cdot \text{LOGN}((P_{\max} + B \cdot 0.5 \cdot solrad \cdot 10^6 / daylength) / P_{\max} + B \cdot 0.5 \cdot solrad \cdot 10^6 \cdot e^{-MK \cdot MLAI} / daylength)), \quad (4.10)$$

where  $M_{phos}$  stands for daily photosynthesis of the maize crop,  $MK$  for light distinction coefficient of the maize canopy (here 0.6),  $MLAI$  for leaf area index of the maize crop,  $B$  for initial solar radiation use efficiency (here  $1.15 \times 10^{-5}$  g CO<sub>2</sub>/J for maize), and  $P_{\max}$  for the maximum photosynthetic rate of leaf, here 6.0 g CO<sub>2</sub>/m<sup>2</sup>·h.

$P_{\max}$  is closely related to temperature, so a temperature-modified form ( $P_t$ ) is

$$P_t = \begin{cases} \frac{Tave - 10}{20 - 10} & 10 \leq Tave \leq 20, \\ \frac{Tave - 20}{30 - 20} & 20 \leq Tave \leq 30, \\ P_{\max} & 30 \leq Tave \leq 40. \end{cases} \quad (4.11)$$

$P_{\max}$  can be modified for availability of soil water and nitrogen in the same way as explained for wheat.

#### 4.2.2 Respiration

The maintenance respiration rate of maize can be calculated by

$$R_m = R_{m0} Q_{10}^{(T-70)/10}, \quad (4.12)$$

where  $Rm$  stands for the maintenance respiration rate at temperature  $T$  in  $\text{g CO}_2/\text{g biomass}\cdot\text{h}$ ,  $Rm_0$  for maintenance respiration rate at temperature  $T_0$  in  $\text{g CO}_2/\text{g biomass}\cdot\text{h}$  and  $Q_{10}$  for temperature coefficient (set at 2).

Assuming  $T_0 = 30^\circ\text{C}$  and  $RM_0 = 0.00125$ , then the total respiration ( $Mrresp$ ) will be

$$Mrresp = 0.00125 \cdot MTb \cdot 2^{((Tave-30)/10)}, \quad (4.13)$$

where  $MTb$  is total biomass of maize. And growth respiration  $Mssresp$  can be calculated by

$$Mssresp = 0.28 Mphos, \quad (4.14)$$

where 0.28 is the respiration coefficient of maize and  $phos$  is the total photosynthesis rate.

#### 4.2.3 Net photosynthetic rate

Daily net photosynthetic rate of maize  $Mnphos$  is the difference between daily total photosynthesis and daily respiration, i.e.,

$$Mnphos = Mphos - (Mrresp + Mssresp). \quad (4.15)$$

## 5 Carbohydrate partitioning and yield formation sub model

### 5.1 Wheat

The ratio of increase in mass of an organ to that of the whole crop, known as partitioning coefficient of the organ (Tong and Cheng, 1997), is calculated as

$$C(d)_i = \frac{MT(d+1)_i - MT(d)_i}{MT(d+1) - MT(d)}, \quad (5.1)$$

where  $C(d)_i$  stands for partitioning coefficient of an organ,  $MT(d+1)_i$  for biomass of an organ at day  $d+1$ ,  $MT(d+1)$  for biomass of the whole crop at day  $d+1$ ,  $MT(d)$  for biomass of the whole crop at day  $d$ , and  $MT(d)_i$  for biomass of an organ at day  $d$ .

As the internal mechanism of carbohydrate partitioning in wheat is not well understood, so individual partitioning coefficients are used in this model for the various phenostages listed in Table 2 (Sinclair and Horie, 1989). Values between phenostages are calculated by linear interpolation. Growth rate of an organ is thus calculated as

$$R(\text{organ}) = C(d)_i \times Nphos. \quad (5.2)$$

Biomass of an organ ( $Worgan$ ) is the integral of growth rate ( $Rorgan$ ) over time, i.e. phenostages, so

$$Worgan = \int_0^n (Rorgan) dt, \quad (5.3)$$

$$Rse = Wleaf \cdot \max\left(0, 1 - \frac{5}{\max(0.01, WLAI)}\right). \quad (5.4)$$

**Table 2** Biomass partitioning coefficients to various organs according to phenostage in winter wheat

Phenostage	Root	Stem	Leaf	Grain
Before winter	0.48	0	0.52	0
During winter	0.3	0.2	0.5	0
Green recovering	0.25	0.26	0.49	0
Stem elongation	0.22	0.34	0.44	0
Booting	0.13	0.52	0.35	0
Heading	0.05	0.82	0.13	0
Flowering	0	0.74	0	0.26
Grain filling	0	-0.34	0	1.34

Note: Biomasses of other parts of the ear except grains are calculated into stem.

Part of the biomass in leaves is lost as leaves die. In this model, death rate of leaves ( $Rse$ ) before booting is calculated with Eq. (5.4) (Bergstrom et al., 1991).

It is assumed that the maximum  $LAI$  a wheat canopy can achieve before booting is 5 (Huang et al., 1996) because extra leaf area would die due to shading. The senescence rate ( $\gamma$ ) increases exponentially with time ( $days$ ) after booting and can be described (Feng, 1995) as

$$\gamma = 0.00435 (days)^{0.882}. \quad (5.5)$$

Thus wheat leaf area index  $WLAI$  can be calculated with

$$WLAI = (Wleaf - Wdeadleaf) \times Wsla, \quad (5.6)$$

where  $Wsla$  is the specific leaf area of wheat (here taken as 0.0235).

Yield arises from the biomass partitioned to fill grains, of which about one third is formed before and two thirds after heading (Jiang and Liang, 1994). Thus grain yield of wheat ( $Wgrain$ ,  $\text{g CH}_2\text{O}/\text{m}^2$ ) can be described as

$$Wgrain = \int_{3.05}^4 Nphos \cdot (-3.207 + 1.137 \cdot Wpheno \log y) dt. \quad (5.7)$$

### 5.2 Maize

In a maize crop carbohydrate is partitioned to the three components of shoots, viz. leaf, stem and grain. Sheaths, cobs, husks and tassels are included in stems. The calculations are as follows (Sun and Hong, 1997):

$$RMroot = \begin{cases} 0.33 \cdot Mnphos & Mpheno < 2, \\ (-0.33 * Mpheno + 0.99) \cdot Mnphos & 2 \leq Mpheno < 3, \\ 0 & Mpheno \geq 3, \end{cases} \quad (5.8)$$

$$RMleaf = \begin{cases} 0.536 \cdot Mphos & Mpheno < 2, \\ (-0.487 \cdot Mpheno + 1.511) \cdot Mnphos & 2 \leq Mpheno < 3.1, \\ 0 & Mpheno \geq 3.1, \end{cases} \quad (5.9)$$

$$RMstem = \begin{cases} 0.134 \cdot Mnphos & Mpheno < 2, \\ (0.787 \cdot Mpheno - 1.441) \cdot Mnphos & 2 \leq Mpheno < 3.1, \\ \left(1 - \frac{Mpheno - 3.1}{0.17}\right) \cdot Mnphos & 3.1 \leq Mpheno < 3.27, \\ 0 & Mpheno \geq 3.27, \end{cases} \quad (5.10)$$

$$RM_{grain} = \begin{cases} 0 & M_{pheno} \leq 3.1, \\ ((M_{pheno} - 3.1) / 0.17) \cdot M_{nphos} & 3.1 \leq M_{pheno} < 3.27, \\ M_{nphos} & M_{pheno} \geq 3.27, \end{cases} \quad (5.11)$$

where  $RM_{root}$  stands for growth rate of roots,  $RM_{leaf}$  for growth rate of leaves,  $RM_{stem}$  for growth rate of stems, and  $RM_{grain}$  for growth rate of grains.

Biomass of individual organs ( $Morgan$ ) is the integral of the organ's growth rate over time, i.e., phenostages

$$Morgan = \int_0^{M_{pheno}} Rorgandt. \quad (5.12)$$

Leaf area index ( $MLAI$ ) of maize is calculated as follows:

$$MLAI = (M_{leaf} - M_{deadleaf}) \cdot M_{sla}, \quad (5.13)$$

where  $M_{leaf}$  stands for the biomass of leaves,  $M_{deadleaf}$  for the biomass of dead leaves, and  $M_{sla}$  for the specific leaf area (here it is 0.0222).

It is assumed that the maximum  $LAI$  that a canopy can achieve before booting is, as for wheat, limited by shading and the value for maize is 3 (Tong and Cheng, 1997). The senescence rate of maize leaves during this stage ( $Rmsene$ ) is thus calculated by

$$Rmsene = M_{leaf} \times \max(0, 1 - 3 / \max(0.001, MLAI)). \quad (5.14)$$

Leaf senescence rate after booting is a function of phenostage that can be represented by

$$Rmsene = M_{leaf} \times 0.000\ 046 \times e^{2.12 \times M_{pheno}}. \quad (5.15)$$

Maize grain yield is mainly determined by the partitioning of carbohydrate after flowering, thus the yield can be calculated by

$$M_{grain} = \int_{3.1}^4 RM_{grain} dt. \quad (5.16)$$

## 6 Soil water balance sub model

The target area of this study is flat and the groundwater is deep below the root zone, so there is no runoff and no access by the crops to groundwater. The field water balance can, therefore, be calculated with

$$W_{i+1} - W_i = R + I - Dn - ET, \quad (6.1)$$

where  $W_{i+1}$  stands for the soil water content at time  $i + 1$ ,  $W_i$  for the soil water content at time  $i$ ,  $R$  for the precipitation,  $I$  for the irrigation,  $Dn$  for the drainage out of the root zone, and  $ET$  for the evapotranspiration.  $R$  is generated with the weather generator; and  $I$  is input into the model as actual

irrigation amounts for specified irrigation strategies, while  $ET$  is calculated with

$$ET = E + T. \quad (6.2)$$

Here,  $E$  stands for soil evaporation and  $T$  crop transpiration.

### 6.1 Soil evaporation and crop transpiration

#### 6.1.1 Potential evaporation and actual evaporation

Potential evaporation  $Ep$  is determined by weather conditions of temperature, humidity and wind speed and can be estimated as

$$Ep = Epan \times 0.8, \quad (6.3)$$

where  $Epan$  is the evaporation from a free water surface (an evaporation pan) at the field site.

The relationship between actual evaporation, the potential evaporation when top soil is saturated, and canopy shading that can be represented as follows (Ritchie et al., 1985):

$$Reva = Ep \cdot e^{-0.8 \cdot LAI}. \quad (6.4)$$

Actual soil evaporation decreases with water content in the top soil according to the coefficient  $Ks$  (Ritchie et al., 1985) that can be calculated as follows:

$$Ks = \ln(Av + 1) / \ln(101), \quad (6.5)$$

$$Av = (W - Wa) / (Wf - Wa) \cdot 100(\%), \quad (6.6)$$

where  $W$  is the soil water content of the top soil layer at 0–30 cm,  $Wa$  is the water content of wind-dry soil sample from the same layer, and  $Wf$  is the field capacity.

Thus, soil evaporation for drying soil can be calculated by

$$Reva(w) = Ep \cdot e^{-0.8 \cdot LAI} \cdot Ks. \quad (6.7)$$

#### 6.1.2 Potential transpiration and actual transpiration

Potential transpiration can be calculated by Eq. (6.8) (Gong, 1994):

$$Tp = 0.9 \times Epan \times 0.8. \quad (6.8)$$

It is assumed in this model that actual transpiration equals to water uptake by root system.

### 6.2 Water uptake rate by root system from component soil layers

On a macro scale, the root system is considered to absorb water from the component soil layers at individual rates (Gong, 1994) using the water-absorbing functions proposed by Novak (1987).

### 6.2.1 Water-absorbing function of wheat root system without water deficit

When the actual transpiration equals potential transpiration, there is no limit to the rate of water flowing into the root system. Under these conditions, the water uptake can be described with the following equation:

$$S_0(z,t) = Tp \cdot \frac{\exp(-\delta \cdot (Zi / Zri))}{Zri(1 - \exp(-\delta))}, \quad (6.9)$$

where  $S_0(z,t)$  is the amount of water taken from an individual unit volume of soil in unit time,  $Tp$  is the potential transpiration,  $Zi$  is the depth of soil layer  $i$ ,  $Zri$  is the depth of root at phenostage  $i$ , and  $\delta$  is an experimental coefficient with value set at 3.01 before winter, 3.53 during "greening" immediately after winter, 3.68 at stem elongation and 3.72 at grain filling.

### 6.2.2 Water-absorbing function of wheat root system under water deficit

Root water uptake is determined by soil resistance, root resistance and evaporation. Soil resistance increases as water content decreases and can be depicted as

$$S = S_0(z,t) \cdot a(\theta), \quad (6.10)$$

where  $a(\theta)$  is the soil resistance to water uptake.

When water content  $\theta$  is below a marginal point  $\theta d$  (Feddes et al., 1979), root water uptake decreases to zero while  $\theta$  reaches the coefficient value. The relation can be depicted as

$$a(\theta) = \begin{cases} 0 & 0 < \theta \leq \theta_w, \\ \frac{\theta - \theta_w}{\theta d - \theta_w} & \theta_w < \theta < \theta d, \\ 1 & \theta d \leq \theta \leq \theta_v, \end{cases} \quad (6.11)$$

where  $\theta d$  is a threshold soil water content below which resistance to root water uptake appears. In this model,  $\theta d$  is set at  $-1$  bar as a soil water content equivalent to water potential.  $\theta_w$  is the wilting soil water content of soil layers.

### 6.2.3 Root water uptake by summer maize

The model of Delong and Cameron (1979) is used to calculate water uptake by the maize root system. It specifies that

$$Smi = Tp \times RD_i / \int_1^n RD_i dz, \quad (6.12)$$

where  $Smi$  is the maximum root water uptake rate from soil layer  $i$ ,  $RD_i$  is the root density at soil layer  $i$ , and  $Tp$  is the potential transpiration during the maize crop growth.

Soil resistance is again represented by  $a(\theta)$ , and  $\theta d$  is assumed to equal to the soil water content when water potential equals to  $-0.8$  bar (You and Wang, 1996).

The distribution of root density in soil layers can be described in the following equation (Gong, 1994)

$$RL(z) = e^{-fz+c}, \quad (6.13)$$

where  $RL(z)$  is the root length at soil depth  $z$ , and  $f$  and  $c$  are correlation coefficients.

Total root length is the integral of root length in the entire root zone, calculated as

$$RL = \int_0^{Zr} e^{-fz+c} dz, \quad (6.14)$$

where  $Zr$  is the maximum depth of root system.

### 6.3 Vertical movement of soil water in root zone

Mono dimensional vertical soil water movement in the root zone can be calculated by ignoring effects of temperature, solutes and hysteresis (Gong, 1994; Hooker and Sander, 1980; Wang, 1999) as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( K(\theta) \frac{\partial \varphi}{\partial z} - 1 \right) - S(z,t), \quad (6.15)$$

where  $\theta$  stands for the soil volume water content,  $\varphi$  for the matric soil water potential,  $K(\theta)$  for the unsaturated soil water conductivity,  $t$  for the time, and  $S(z,t)$  for the water-absorbing function of root system.

## 7 Soil nitrogen sub model

### 7.1 Soil nitrogen balance and convection-dispersion equations

Both balance equations and mechanic models are used to simulate soil nitrogen dynamics. Soil nitrogen balance can be represented in Eq. (7.1) (Aslyng, 1985):

$$\Delta N_i = N_a + N_f + N_m - N_d - N_i - N_u, \quad (7.1)$$

where  $\Delta N_i$  stands for the change of soil inorganic nitrogen over time,  $N_a$  for the nitrogen input from rainfall and biological fixation,  $N_f$  for the nitrogen input in fertilization,  $N_m$  for the nitrogen supply by mineralization of organic matter,  $N_d$  for the denitrification,  $N_i$  for the amount of organic nitrogen leached to the lower soil layer or transferred to upper soil layer, and  $N_u$  for the crop uptake.

$\text{NH}_4\text{-N}$  is ignored in this model because its content in dryland soils is usually very small (Aslyng, 1985).  $\text{NO}_3\text{-N}$ , on the other hand, is very mobile in the irrigated soil and is depicted with a mono-dimensional dynamic equation (Hooker and Sander 1980, Aslyng 1985) as

$$\frac{\partial(\theta \cdot C)}{\partial t} = \frac{\partial}{\partial z} \left[ Dsh(\theta, v) \cdot \frac{\partial C}{\partial z} \right] \cdot \frac{\partial(qC)}{\partial z} + \varphi(z,t), \quad (7.2)$$

where  $C$  stands for the  $\text{NO}_3\text{-N}$  content in soil solution,  $Z$  for the soil depth,  $\theta$  for the volume soil water content,  $t$  for the time,  $Dsh(\theta, v)$  for the convection-dispersion coefficient of  $\text{NO}_3\text{-N}$  in the soil, and  $\varphi(z, t)$  for the whole process of soil nitrogen transfer including crop uptake.

## 7.2 Estimation of coefficients relating to nitrogen transfer and movement

### 7.2.1 Convection-dispersion coefficient of $\text{NO}_3\text{-N}$

The convection-dispersion coefficient ( $Dsh$ ,  $\text{cm}^2/\text{d}$ ) is divided into two parts (Ju, 2000): convection  $Dn$  and dispersion  $Dh$ , then

$$Dsh = Dn + Dh, \quad (7.3)$$

$$Dn = D_o \cdot a \cdot e^{b\theta}, \quad (7.4)$$

$$Dh = n \cdot |v|, \quad (7.5)$$

where  $D_o$  stands for the dispersion coefficient of the ions in water ( $\text{cm}^2/\text{d}$ ),  $V$  for the mean porous flow rate ( $\text{cm}^2/\text{d}$ ), and  $a$ ,  $b$  and  $n$  for the empirical coefficients. Some coefficient values are shown in Table 3.

**Table 3** Coefficients for estimating convection-dispersion coefficient of  $\text{NO}_3\text{-N}$

Soil depth (cm)	$a$	$b$	$n$
0–65	0.24	10	0.32
65–120	0.058	10	0.22
120–160	0.058	10	0.22
160–200	0.24	10	0.32

### 7.2.2 Coefficient of nitrogen transfer

This model considers only mineralization, fixation and denitrification, and those in response to temperature and moisture content. Taking  $KK_{opt}$  as the rate coefficient in a transfer process at optimal temperature  $T_{opt}$  and moisture content  $\theta_{opt}$ , then the coefficient  $KK$  under specific temperature and moisture content can be calculated by

$$KK = KK_{opt} \times a(T - T_{opt}) \times \theta_{opt} / \theta \quad \text{when } \theta \geq \theta_{opt}, \quad (7.6)$$

$$KK = KK_{opt} \times a(T - T_{opt}) \times \theta / \theta_{opt} \quad \text{when } \theta < \theta_{opt}, \quad (7.7)$$

where  $a$  stands for an empirical coefficient.

The above method is suited for mineralization and fixation, and the denitrification is more appropriately adjusted with the equation

$$KK = KK_{opt} \times a(T - T_{opt}) \times (\theta - \theta_1) / (\theta_{opt} - \theta_1), \quad (7.8)$$

where  $\theta_1$  stands for the lower limit of moisture content for denitrification, usually taking a value of 0.15 (Zhao, 1999). Denitrification does not occur when moisture content is less than  $\theta_1$ .

## 7.3 Simulation of soil temperature

Daily average soil temperature  $ST(z)$  of individual soil layers is calculated with the method used in CERES-Maize (Huang et al., 1996) as follows:

$$ST(z) = TAV + (AMP \times \text{COS}(ALX + ZD)/2 + DT) \times e^{zD}, \quad (7.9)$$

where  $TAV$  stands for the annual average air temperature at the field site,  $AMP$  for the annual difference of daily average air temperature at the field site,  $ALX$  for the radian of the calculated date over a year,  $ZD$  for the factor that temperature decreases as soil layer goes deeper, and  $DT$  for the difference of actual surface soil temperature over time ( $^\circ\text{C}$ ).

## 8 Nitrogen uptake and allocation

### 8.1 Function of root nitrogen uptake

Root nitrogen uptake is affected by soil nitrogen content and moisture regime in addition to climatic factors and cultivars. The Michaelis-Menten equation is used to simulate root nitrogen uptake from individual soil layers (Wang and Li, 1999), represented as

$$f_i(T) = B \cdot f_{pp} \left( \frac{t}{T} \right) \cdot \frac{[\text{NO}_3^-]_i}{[\text{NO}_3^-]_i + K_{ab}} \cdot \frac{RD_i}{\int_1^N RD_i dz} \cdot f(w), \quad (8.1)$$

where  $f_i(T)$  stands for the rate of root nitrogen uptake in layer  $i$  ( $\text{kg}/\text{hm}^2 \cdot \text{d}$ ),  $i$  for soil depth,  $N$  for the number of soil layers that the root system can penetrate,  $B$  for potential crop nitrogen uptake ( $\text{kg}/\text{hm}^2$ ),  $f_{pp}(t/T)$  for the resistance coefficient, i.e. the quotient of daily nitrogen uptake over total nitrogen uptake,  $t$  for the number of days after sowing,  $T$  for the crop growth period, i.e. the number of days from sowing to maturity,  $RD_i$  for the root length density in soil layer  $i$  ( $\text{cm} \cdot \text{cm}^{-3}$ ),  $[\text{NO}_3^-]_i$  is  $\text{NO}_3\text{-N}$  content ( $\text{mg}/\text{kg}$ ) in soil solution from layer  $i$ ,  $f(w)$  for the factor of soil moisture effect, and  $K_{ab}$  for the Michaelis-Menten constant.

Soil moisture content determines movement and accumulation of ions. Under the low water content, movement is restricted while the high water content can decrease the potential and hence the actual crop nitrogen uptake. In this model, crop nitrogen uptake is modified as follows:

$$f(w) = 0.5 \quad \text{when soil water potential} < -0.9 \text{ MPa, and}$$

$$f(w) = 0.8 \quad \text{when soil water potential} > -0.01 \text{ Mpa.}$$

The Michaelis-Menten constant  $K_{ab}$  takes either of two values according to growth stage as listed for wheat and maize in Table 4 (Huang et al., 1996).

### 8.2 Crop nitrogen demand and coefficient of nitrogen sufficiency

The maximum nitrogen demand of a crop is defined as the nitrogen content (%) of the whole plant biomass for the crop

**Table 4**  $K_{ab}$  values of wheat and maize (mg/kg)

Growth stage		$K_{ab}$		
Emergence-flowering	Winter wheat	30	Summer maize	0.5
Flowering-maturity		40		1.5

to achieve maximum growth under optimum conditions. It is determined by genetic factors so it is related only to the stages of development. The maximum nitrogen demands of wheat above-ground and underground parts can be calculated with Eqs. (8.2) and (8.3) respectively:

$$TCNP = (-4.8112 - 6.5507 \cdot Zstage + 15.9578 \cdot \sqrt{Zstage} + 0.2138 \cdot Zstage^2) / 100, \quad (8.2)$$

$$RCNP = (1.8 - 0.17 \cdot \sqrt{Zstage}) / 100. \quad (8.3)$$

In the above equations,  $Zstage$  is the development index in Zadok's Scale (Sinclair and Horie, 1989). And the values for various phenostages are estimated by

$$Zstage = \begin{cases} 0 & phenostage < 1, \\ 2 \cdot (phenostage - 1) & 1 \leq phenostage \leq 2, \\ 2 + 4.348 \cdot (phenostage - 2) & 2 < phenostage \leq 2.46, \\ 4 + 3.184 \cdot (phenostage - 2.46) & 2.46 < phenostage \leq 3, \\ 5.7 + 4.57 \cdot (phenostage - 3) & 3 < phenostage \leq 3.07, \\ 6.02 + 3.135 \cdot (phenostage - 3.07) & 3.07 < phenostage \leq 4. \end{cases} \quad (8.4)$$

The minimum crop nitrogen demand is defined as the minimum nitrogen content available for plant growth. The minimum nitrogen demand of above-ground organs ( $TMNC$ ) is one third of the maximum nitrogen demand (Zhao, 1999; Sun and Hong, 1997), i.e.,

$$TMNC = TCNP/3. \quad (8.5)$$

The actual nitrogen content of above-ground organs ( $TANC$ ) is calculated as follows:

$$TANC = \frac{(LeafN + StemN + GrainN)}{(Wleaf + Wstem + Wgrain)}, \quad (8.6)$$

where  $leafN$ ,  $StemN$  and  $GrainN$  stand for the measured nitrogen contents in leaves, stems and grains, respectively in g/m<sup>2</sup>.

The nitrogen sufficiency index  $NFAC$ , which affects crop growth and development, can be calculated by Eq. (8.7) (Sun and Hong, 1997):

$$NFAC = \min(1, (TANC - TMNC) / (TCNP - TMNC)). \quad (8.7)$$

### 8.3 Daily nitrogen demand, uptake and partition to various organs

It is assumed in this model that the nitrogen uptake begins at emergence and ceases at flowering when root senescence begins. Most of the nitrogen for grain-filling is transferred

from vegetative organs (Feng, 1995; Garry et al., 1996; Aggarwal and Naveen, 1994; Wang and Wang, 1989).

Daily nitrogen demand of a crop organ is determined by daily maximum nitrogen demand ( $CNP_{(i)}$ ), actual nitrogen content  $N\%$  and biomass  $W_{(i)}$  (Garry et al., 1996), so

$$RneedN_{(i)} = (CNP_{(i)} - (i)N\%) \cdot W_{(i)}, \quad (8.8)$$

where  $i = 1, 2, 3, 4$ , stands for root, stem, leaf and grain, respectively.

Values of  $CNP_{(i)}$  as listed in Tables 5 and 6 are determined empirically (Zhao, 1999; Greenwood, 1988).

**Table 5** Maximum nitrogen demand of wheat organs at various phenostages (% dry weight)

	Root	Stem	Leaf	Grain
Seedling	3	4	6	–
Flowering	1	2	3.5	3
Maturity	0.5	0.3	1	2.75

**Table 6** Maximum nitrogen demand of maize organs at different phenostages (% dry weight)

	Root	Stem	leaf	Grain
Seedling	3	4	6	–
Tasseling	1	2	3.5	3.11
Maturity	0.5	0.4	1	2.68

Before flowering, crop daily nitrogen uptake ( $RuptakeN$ ) is determined by daily nitrogen demand and nitrogen availability ( $\sum RneedN_{(i)}$ ) in the root zone and the uptake is partitioned to various organs according to daily nitrogen demand (Garry et al., 1996; Aggarwal and Naveen, 1994; Wang and Wang, 1989). The difference between nitrogen demand and uptake, and the deficit of nitrogen, may reduce crop growth. Daily nitrogen uptake by vegetative organs can be calculated with

$$RuptakeN = \min \left( \sum_{i=1}^3 RneedN_{(i)}, RootzoneAN \right). \quad (8.9)$$

Daily nitrogen uptake by individual organs can be calculated with

$$RuptakeN_{(i)} = \frac{RneedN_{(i)}}{\sum RneedN_{(i)}} \cdot RuptakeN. \quad (8.10)$$

### 8.4 Nitrogen transfer and accumulation in grains

During the period from flowering to maturity, nitrogen in cell can be transferred into grains, but not in structural tissues (Wang and Lu, 1993). The rate of the transfer from a vegetative organ ( $RtN_{(i)}$ ) can be calculated with Eq. (8.11) (Greenwood, 1988) as follows:

$$RtN_{(i)} = bW(i) \cdot (b[N]_{(i)} - \min[N]_{(i)}) \cdot DTT / \sum T_{(B-M)}, \quad (8.11)$$

where  $bW_{(t)}$  stands for the organ biomass at flowering,  $b[N]_{(t)}$  for the nitrogen content,  $\min[N]_{(t)}$  for the minimum nitrogen demand of organs, and  $DTT$  and  $\sum T_{(B-M)}$  for daily degree days and total degree days during the period of flowering to maturity, respectively.

In this model, nitrogen transferred from vegetative organs is stored in a virtual pool ( $N_{pool}$ ). The actual nitrogen absorption by grains ( $R_{grainN}$ ) can be determined by the lesser daily nitrogen demand ( $R_{needN_d}$ ) and the size of  $N_{pool}$ .  $R_{grainN}$  can also be affected by a nitrogen sufficiency coefficient of the above-ground parts. Those relations are depicted in Eq. (8.12):

$$R_{grainN} = NFAC \times \min(N_{pool}, R_{needN_d}) \quad (8.12)$$

## 8.5 Crop nitrogen loss

Crop nitrogen loss includes the nitrogen removed in dead tissues and gaseous loss after flowering (Greenwood 1988; Sinclair and Amir, 1992). The nitrogen is lost only in dead leaves, as the dominant way of nitrogen loss, which can be calculated in this model. Rate of nitrogen loss ( $R_{dieleafN}$ ) can be depicted with Eq. (8.13) as

$$R_{dieleafN} = \begin{cases} R_{dieleaf} \cdot LeafN\% & LeafN\% > 0.025, \\ R_{dieleaf} \cdot 0.01 & LeafN\% \leq 0.025, \end{cases} \quad (8.13)$$

where  $LeafN\%$  stands for the nitrogen content of dry mass of leaf and 0.01 is an empirical coefficient.

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