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A universal agro-hydrological model for water and nitrogen cycles in the soil-crop system SMCR_N: critical update and further validation

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Abstract

Agro-hydrological models have widely been used for optimising resources use and minimizing environmental consequences in agriculture. SMCR_N is a recently developed sophisticated model which simulates crop response to nitrogen fertilizer for a wide range of crops, and the associated leaching of nitrate from arable soils. In this paper, we describe the improvements of this model by replacing the existing approximate hydrological cascade algorithm with a new simple and explicit algorithm for the basic soil water flow equation, which not only enhanced the model performance in hydrological simulation, but also was essential to extend the model application to the situations where the capillary flow is important. As a result, the updated SMCR_N model could be used for more accurate study of water dynamics in the soil-crop system. The success of the model update was demonstrated by the simulated results that the updated model consistently out-performed the original model in drainage simulations and in predicting time course soil water content in different layers in the soil-wheat system. Tests of the updated SMCR_N model against data from 4 field crop experiments showed that crop nitrogen offtakes and soil mineral nitrogen in the top 90 cm were in a good agreement with the measured values, indicating that the model could make more reliable predictions of nitrogen fate in the crop-soil system, and thus provides a useful platform to assess the impacts of nitrogen fertilizer on crop yield and nitrogen leaching from different production systems.

Key words: soil-crop system, modeling, water and nitrogen transfer, agricultural water management, nitrogen management, nitrogen leaching.

1. Introduction

Agro-hydrological models have proved to be useful tools in optimizing irrigation scheduling and fertilizer application, and in assessing the impact of different farming practices on the environment. Numerous models for various crop species have been reported for these purposes in the literature in the last few decades (Johnsson et al., 1987; Bergstrom et al., 1991; Williams et al., 1993; Diekkruger et al., 1995; Hoogenboom et al., 1999; Brisson et al., 2003; Jones et al., 2003; Keating et al., 2003; Stöckle et al., 2003; van Ittersum et al., 2003; Zhang et al., 2007, 2009; Rahn et al., 2010).

A large number of agro-hydrological models are devoted to assessing the effects of nitrogen (N) fertilizer on crop growth and N leaching for various crop species (see the review by Cannavo et al., 2008). The most prominent models that cover a range of crops are the EPIC models (Williams et al., 1993) and the DSSAT models (Hoogenboom et al., 1999). Although the EPIC and DSSAT models have proved useful in both basic and applied studies of the effects of climate and management on growth and the environment, the models are generally crop specific, and require parameter values which are difficult to determine for a given crop. Lack of generality is a common feature for crop N models. According to the recent review by Cannavo et al. (2008) where 62 crop N models were surveyed, only 2 models are able to simulate the N cycle for 4 crops families, while a vast majority of the models are only able to deal with a single crop, mainly cereal crops. This has caused difficulties in the use of models for optimizing N inputs in crop production where various crops are grown. Developing generic models which are able to assess the effects of N fertilizer on crop growth and the associated N leaching is evidently important.

A new crop N model named SMCR_N model, which is based on a version of N_ABLE (Greenwood, 2001) and EU-Rotate_N (Rahn et al., 2010), has been developed for crop N response and N leaching in arable soils (Zhang et al., 2009). The model covers a wide range of crops, which makes it a good candidate for forecasting both optimum N inputs and the environmental consequences of crop production. Compared with most models of its kind, the SMCR_N model is much more mechanistically based. A promising degree of agreement was found between predictions of the SMCR_N model and actual measurements of responses of crop yield and N mineral composition to N fertilizer from 32 field experiments over 16 crops (Zhang et al., 2009). However, the model at present uses an approximate cascade type of algorithm to calculate the redistribution of water and nitrate and losses by percolation and leaching from the soil profile. Although this approach is simple and easy to implement, it is unable to simulate capillary flow and can give poor predictions of daily soil water changes (Gandolfi et al., 2006; Cannavo et al., 2008; Yang et al., 2009). It is therefore unsatisfactory for some circumstances including those where the groundwater table is high and thus upward capillary flow can largely satisfy demands of evapotranspiration (Yang et al., 2009). Moreover, it is difficult to implement boundary conditions precisely at the lower boundary in the cascade model, which could result in unreliable predictions as the hydrological simulations are highly sensitive to the parameterization at the lower boundary (Boone and Wetzel, 1996).

It is well known that a numerical approach using the Richards' equation could simulate soil water movement more accurately. Such a basic theory of water movement in soil is now widely accepted but, despite substantial advances in mathematics and computer science, the uptake of models of this type is still low (Bastiaanssen et al. 2007). One reason for this is the complex nature of the numerical methods involved, and the resulting long program code. In spite of the fact that the numerical schemes such as the finite element (FE) method for solution to the Richards' equation are well developed (Šimunek et al., 1992), their use requires specialized expertise that many potential users have not got. This has led to the adoption of cascade method for soil water movement in many agro-hydrological models on fertilizer, irrigation and pesticide practices. For example, Cannavo et al. (2008) found that a large proportion of crop N models (7 out of 16) adapted the cascade approach for hydrological simulations, while Ranatunga et al. (2008) reported that the majority of soil water models (13 out of 21) that have been widely applied in Australia using a similar method. In order to address this problem, a promising alternative algorithm, based on the work by Lee and Abriola (1999), has been proposed to simulate water dynamics in the soil-crop system where the Richards' equation was employed for the description of soil water movement (Yang et al., 2009). The algorithm considers that the water content in a soil layer in a small time step of 0.001 d is only influenced by its adjacent layers, i.e. those immediately above and below. It has been demonstrated that the simple and explicit algorithm could accurately reproduce the spatial-temporal soil water content in the cropped soils (Yang et al., 2009).

The primary objectives of the study include: 1) update the SMCR_N model (Zhang et al., 2009) with the recently developed simple and highly accurate algorithm (Yang et al., 2009) for hydrological simulations; 2) to compare the simulated values of soil water distribution made by the updated model, the original model, and the highly accurate FE procedure in modeling water drainage in contrasting soils; 3) to compare the performance of the updated SMCR_N model with the original version in predicting soil water dynamics in the soil-wheat system; 4) to validate the updated SMCR_N model against data of crop N and soil mineral-N from new field experiments on 4 different crops.

2. The model

2.1. Model framework

The SMCR_N model (Zhang et al., 2009) operates on uniform 5 cm soil layers that are widely used in the agro-hydrological models to describe processes such as root length distribution in the soil-crop system (Greenwood, 2001, Zhang et al., 2007, Renaud et al., 2008, Yang et al., 2009; Pedersen et al., 2010; Rahn et al., 2010). It is not our intention to present a detailed description of the whole model here since the SMCR_N model has been published (Zhang et al., 2009). Instead we focus on the modifications to the model, i.e. the new hydrology module, and its performance in simulating soil water drainage and soil water dynamics in the soil-crop system. We also focus on the validation of the updated model against data from new field experiments. However, to help to understand the model framework, we provide the schematic representation of the updated SMCR_N model (Fig. 1), a brief description of the principles and the key equations included in the other major modules. The justification of employing the equations in these modules can be seen in Zhang et al. (2009).

The updated model differs from its predecessor in that two time steps are employed. The model calculates plant dry matter accumulation, root length distribution, potential evaporation, and potential N and water requirements for plant growth on a daily basis, whereas a much smaller time step of 0.001 d is implemented in the algorithms for calculating actual soil evaporation, water and N uptake by roots, and soil water and N movement. The implementation of such procedures is similar with that for modeling water transfer in the soil-crop system (Yang et al., 2009).

2.2 Hydrology module

In a 1-D situation, the Richards' equation governing water flow under gravity in an isotropic variably saturated soil is (Celia et al. 1990; Šimunek et al., 1992; Zhang et al., 2010):

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}[K(\theta)(\frac{\partial h}{\partial z}+1)] \tag{1}$$

where θ (cm^3 cm^{-3}) is the volumetric soil water content, t (d) is time, K (cm d^{-1}) is the soil hydraulic conductivity, h (cm) is the soil pressure head, and z (cm) is the vertical coordinate.

The soil hydraulic functions are defined according to van Genuchten (1980) and Mualem (1976):

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = [\frac{1}{1 + |\alpha h|^n}]^m \tag{2}$$

$$K(\theta) = K_s \Theta^{0.5} [1 - (1 - \Theta^{1/m})^m]^2 \tag{3}$$

where Θ is the relative saturation, θ_s and θ_r (cm^3 cm^{-3}) are the saturated and residual soil water contents, α (cm^{-1}) and *n* are the shape parameters of the retention and conductivity functions, *m*=1-1/*n*, and K_s (cm d^{-1}) is the saturated hydraulic conductivity.

Integrating Eq. (1) vertically over a soil layer leads to (Lee and Abriola, 1999; Yang et al., 2009):

$$\frac{\Delta \overline{\theta_i}}{\Delta t} = \frac{1}{\Delta z}(w_{i+1} - w_i) \tag{4}$$

where

$$w_i = K_i (\frac{\Delta h_i - \Delta h_{i-1}}{\Delta z} + 1) \tag{5}$$

in which *i* is the soil layer number, numbered from 1 at the bottom layer of the profile and increasing upwards to the surface layer, Δt (d) is the time step, Δz (cm) is the soil layer thickness, w_{i+1},w_i (cm d^{-1}) are the water fluxes from layer *i+1* to *i*, and *i* to *i-1*, respectively, $\Delta\overline{\theta_i}$ (cm^3 cm^{-3}) is the layer-average soil water content change in layer *i* in Δt, and Δh_i and Δh_{i-1} (cm) are the soil pressure head in the layers *i* and *i*-1, respectively.

When rainfall plus irrigation are greater than the potential evaporation, the water flux from the surface is considered as infiltration. The actual infiltration flux, ΔI_{act} (cm d^{-1}), is determined by the following equation (Yang et al., 2009):

$$\Delta I_{act} = \min\{K_s, \min[(\theta_s - \theta_{Top})\Delta z / \Delta t, R]\} \tag{6}$$

in which R (cm d^{-1}) is the possible net water flux at the surface, and θ_{Top} is the water content in the top soil layer.

If the potential evaporation exceeds the sum of rainfall and irrigation, the actual evaporation in a given time step from the top soil layer, ΔE_{act} (cm d^{-1}), is expressed as (Yang et al., 2009):

$$\Delta E_{act} = \min\{K_{Top}[(h_{\min} - h_{Top})/\Delta z + 1], R\} \tag{7}$$

where K_{Top} (cm d^{-1}) and h_{Top} (cm) are the hydraulic conductivity and soil pressure head in the top layer, respectively, and h_{min} (cm) is the minimum soil pressure head that the atmosphere could possibly exert in the top soil layer, equal to the soil pressure head corresponding to half water content at the permanent wilting point as recommended by the FAO (Allen et al., 1998).

The treatment of N transport in the soil is simple. The proportion of N transported from a soil layer is considered to be identical to the ratio of water drainage out of the layer to the total water in the layer (Burns, 1974; Greenwood, 2001; Zhang et al., 2007, 2009; Pedersen et al., 2010). Diffusion terms for N transport in the soil are not included in the simulation.

2.3 Plant growth module

The actual daily increments in plant dry weight excluding the fibrous roots are calculated by a growth equation which allows the crop to grow exponentially in the early growth stages and linearly towards maturity (Greenwood, 2001; Zhang et al., 2007, 2009).

$$\Delta W = \frac{K_2 W}{K_1 + W} \times \min\left(\frac{\%N}{\%N_{crit}}, 1\right) \qquad (8)$$

where ΔW (t ha^{-1}) is the maximum possible increment in growth on the day, W (t ha^{-1}) is the dry weight of the entire plant excluding fibrous roots, K_1 (=1 t ha^{-1}) is the semi-maximum W for growth rate, K_2 (t ha^{-1} d^{-1}) is a growth rate coefficient, which can be calculated using the specified target yield, the dry weight at planting and daily mean air temperature (Zhang et al., 2009), %N is the percentage of N in W, $\%N_{crit}$ is the critical %N, i.e. the minimum %N at which growth proceeds at the maximum rate, which is defined by (Greenwood, 2001):

$$\%N_{crit} = \alpha_N (1 + \beta_N e^{-0.26W}) \quad (9)$$

where α_N and β_N are crop specific parameters that relate critical %N to crop dry weight.

In the case of crop capable of luxury N consumption, the possible maximum crop %N in the plant is calculated as follows:

$$\%N_{\max} = R_{lux} \times \%N_{crit} \quad (10)$$

where R_{lux} is the coefficient of crop luxury N consumption.

The increment in root dry weight ΔW_r is considered as a function of the increment in crop dry weight ΔW, crop dry weight W, and a parameter defining root class (Zhang et al., 2009; Pedersen et al., 2010). The total root length is calculated from a fixed specific root length and root dry weight W_r. The root penetration down the soil profile is driven by the accumulative daily mean air temperature. The root length declines logarithmically from the soil surface downwards (Pedersen et al., 2010).

$$R_z = \min\{R_{z0} + \max[0, (\sum T - T_{lag})K_{rz}], R_{z\max}\} \quad (11)$$

$$L(z) = \begin{cases} L_0 e^{-a_z z} & z < R_z \\ L_0 e^{-a_z z}(1 - \dfrac{z - R_z}{0.3R_z}) & R_z \le z \le 1.3R_z \end{cases} \quad (12)$$

where R_z (m) is the simulated rooting depth, R_{z0} (m) is the starting rooting depth, $\sum T$ (^{o}C d) is the cumulative day degree, T_{lag} (^{o}C d) is the threshold of cumulative day degree for root growth, K_{rz} (m day^{-1} °C^{-1}) is the root growth rate, R_{zmax} (m) is the maximum rooting depth restricted by physical barriers, L_0 (m m^{-3}) is the total root length, and a_z is the shape parameter controlling root distribution down the profile. More information about modeling root development is given elsewhere (Pedersen et al., 2010).

2.4 N and water requirements module

Crops are considered to have two N compartments: a top N compartment and a root N compartment (Zhang et al., 2009). The top N compartment contains N of the entire plant excluding N in fibrous roots, whereas the root N compartment stores N allocated in fibrous roots. The demands of N in the top and root compartments are calculated as (Zhang et al., 2009):

$$U_N = 10[(W + \Delta W) \times \%N_{\max} - W \times \%N] \tag{13}$$

$$U_{Nr} = 10[(W_r + \Delta W_r) \times \%N_{rpot} - W_r \times \%N_r] \tag{14}$$

where U_N and U_{Nr} (kg N ha^{-1}) are the potential N uptake in the top and root compartments, respectively, $\%N_r$ is the actual %N in W_r, and $\%N_{rpot}$ is the root potential %N, which is calculated from (Zhang et al., 2009):

$$\%N_{rpot} = 1 + \beta_N e^{-0.26W} \tag{15}$$

The potential soil evaporation and plant transpiration are calculated according to the FAO 56 crop coefficient method (Allen et al., 1998):

$$E_{pot} = K_e ET_0 \tag{16}$$

$$T_{pot} = K_{cb} ET_0 \tag{17}$$

where E_{pot} and T_{pot} are the potential soil evaporation and plant transpiration, respectively, K_e is the evaporation coefficient, K_{cb}, dependent on crop species and its development stage, is the basal crop coefficient for transpiration, ET_0 (mm) is the reference evapotranspiration. ET_0, K_{cb}, K_{cmax} and f can be determined according to Allen et al. (1998).

2.5 N and water uptake module

N uptake is calculated according to crop N demand, root length distribution, soil mineral N concentration and the minimum soil mineral N concentration for root uptake, as proposed by Pedersen et al. (2010).

$$N_{act} = (U_N + U_{Nr})(1 - e^{-\frac{N_{pot}}{U_N + U_{Nr}}}) \tag{18}$$

in which

$$N_{pot} = \Sigma \frac{L(z) k_N (c_N - c_{N\min})}{c_N + c_0} \tag{19}$$

where N_{act} (kg N ha^{-1}) and N_{pot} (kg N ha^{-1}) are the actual and potential N uptake, respectively, c_N (kg N m^{-3}) is the soil mineral N concentration in soil layer, c_{Nmin} (kg N m^{-3}) is the minimum soil mineral N concentration, c_0 (kg N m^{-3}) is the plant N uptake coefficient, and k_N is the plant N uptake efficiency (Pedersen et al., 2010).

The actual crop transpiration T_{act} (cm d^{-1}) is the sum of root water uptake from different layers. It is formulated (Zhang et al., 2009, 2010),

$$T_{act} = \Sigma \alpha_w(h) L(z) T_{pot} / \Sigma L(z) \tag{20}$$

in which

$$\alpha_w(h) = \begin{cases} 0 & h \le h_3\ ,\ h \ge h_1 \\ (h - h_3)/(h_2 - h_3) & h_3 < h < h_2 \\ 1 & h_2 \le h < h_1 \end{cases} \tag{21}$$

where α_w is the root water stress reduction factor. Root water uptake is assumed to be zero when soil pressure head is below h_3, i.e. the soil pressure head at the permanent wilting point (h_3 = -15000 cm), and is unlimited for soil pressure head between h_1 (-1 cm) and h_2^{high} (-500 cm) for a rapid transpiration (0.5 cm d^{-1}) and h_2^{low} (-1100 cm) for a slow transpiration (0.1 cm d^{-1}). The increase in water uptake between h_3 and h_2 is linearly related to the soil pressure head. Water uptake is also assumed to be 0 for soil pressure head greater h_1 due to lack of oxygen in the root zone (Zhang et al., 2009, 2010).

2.6 N mineralization module

N mineralization from soil organic matter is considered in the model. The algorithm is devised based on the assumption that the organic matter breakdown rate is a first-order process. Daily N mineralization from soil organic matter is estimated as follows (Zhang et al., 2009).

$$N_{s\min} = k_{\min} Q_{10}^{\frac{T-T_s}{10}} \rho_s Z_{s\min} \frac{m_c}{R_{CN}} \times 10^5 \tag{22}$$

where N_{smin} (kg ha^{-1}) is the daily N mineralization rate from soil organic matter, k_{min} (d^{-1}) is the temperature-independent coefficient for the rate of organic matter oxidation, $Q_{10}^{\frac{T-T_s}{10}}$ is the correction factor of temperature on N mineralization, ρ_s (g cm^{-3}) is the soil bulk density, Z_{smin} (cm) is the soil depth where N mineralization takes place, m_C (%) is the soil organic C content, R_{CN} is the C:N ratio of the soil organic matter, T_s (^{o}C) is the base temperature at which $Q_{10}^{\frac{T-T_s}{10}}$ equals 1, and Q_{10} is the factor change in rate with a 10 degree change in temperature.

3. Experiments

Experiments on two sites are described in this section. The results of an experiment (PAGV experiment) carried out at the Institute for Soil Fertility Research, Netherlands (Groot and Verberne, 1991) are used to compare the updated and the original versions of the SMCR_N model in simulating water dynamics in the soil-crop system, while the experiments (HRI experiments) conducted at Warwick-HRI, Warwick University, UK are used for the validation of the updated model.

3.1 PAGV experiment for model comparison

The experiment used in model comparison between the updated and the original versions was conducted in the PAGV farm with winter wheat at the Institute for Soil Fertility Research, Netherlands in 1984 (Groot and Verberne, 1991). The crop was sown on 21 October, 1983 and harvested on 21 August, 1984. The soil in the PAGV farm was silty loam. The measurements of soil water in the layers of 0-20, 20-40, 40-60, 60-80 and 80-100 cm were made at intervals of three weeks from 14 February, 1984. Also the time-course of groundwater tables were measured. Detailed description of the experiment and measured weather and soil water data can be seen in Groot and Verberne (1991).

3.2 HRI experiments for model validation

To validate the updated model, field experiments with four contrasting crops were carried out using a completely randomized design on a sandy loam soil at Wellesbourne, Warwick-HRI, UK in 2006. The crops were radish (grown over a very short period and had a small yield), lettuce and cabbage (grown over longer periods and had reasonable yields), and soyabean (a legume and able to fix atmospheric-N). Radish and soyabean were drilled directly, whereas lettuce and cabbage were transplanted using plants raised separately in peat blocks. The experimental plots were 1.52 m x 4 m for cabbage and radish, 1.52 m x 0.6 m for lettuce and 3 m x 4 m for soyabean. For each crop plants were grown in 3 different plots. N fertiliser was broadcast (as NH_4NO_3) at a rate of 100 kg N ha^{-1} on all plots and incorporated to a depth of 10 cm before drilling or transplanting; a further 200 kg N ha^{-1} was top dressed for cabbage at a later date. Applications of other major nutrients, and weed and pest control measures followed normal practice. Further cropping data and other details of the experiments are summarised in Table 1. Three replicate plants from each plot of each crop were randomly selected and harvested at maturity in the end of the experiments. Sub-samples were dried at 80^{o}C to constant weight and then analysed for %N (CN-2000, LECO).

Pre-planting soil samples were taken for mineral N to a 30 cm depth on 5 December 2005 for lettuce and radish, and on 6 February 2006 for cabbage and soyabean, respectively. After harvesting, further soil samples were taken to 90 cm depth on 31 January 2007 for cabbage, 7 February 2007 for soyabean, and 19 February 2007 for lettuce and radish, respectively.

4. Model parameterization

The study was carried out in two parts. In the first part, the performance of the updated model against the original model in hydrological simulations was carried out. This was done by running the models for water drainage in contrasting soils via a numerical experiment, and for soil water dynamics in the PAGV experiment. The results were compared against these from an alternative method and the measurements. The second part involved comparing the predictions of the updated SMCR_N model with the data from the field experiments (HRI experiments) in order to validate it.

4.1 Numerical and PAGV experiments for model comparison

4.1.1 Numerical experiment

To examine how the new hydrology module performed in simulating water drainage in soil columns, it was compared with two alternative methods, i.e. the cascade method originally employed in the SMCR_N model and the highly accurate FE method for solving the soil water flow equation. The simulations were carried out on two contrasting soils: a very coarse soil and a very fine soil. The parameters describing water characteristics for both soils were set to those suggested by Wösten et al. (1999) (see Table 2 for details). The soil columns were assumed to have a depth of 2 m, with an initial soil water content set at saturation throughout the column. The lower boundary condition was specified as free drainage, whereas no water flux was allowed at the surface. In the updated model, the soil column was divided into 40 uniform 5 cm layers, with a simulation time step for both soils of 0.001 d, similar to that proposed by Lee and Abriola (1999) and Yang et al. (2009). In the FE model (Šimunek et al., 1992), the soil domain was divided into 50 soil layers with various thicknesses (thin layers at the bottom where the lower boundary condition was imposed). In the cascade algorithm in the original SMCR_N model, the division of soil column was the same as that in the updated model, i.e. 5 cm each. Drainage occurred only when soil water content exceeded its field capacity. The drainage coefficient was calculated as the ratio of the difference between volumetric soil water contents at saturation and field capacity, to the soil water content at saturation, and the time step was 1 d (Zhang et al., 2009).

4.1.2 PAGV experiment

Soil water retention curves for the PAGV experiment (0-25, 25-40 and 40-100 cm) were measured (Groot and Verberne, 1991). The van Genuchten soil hydraulic property parameters (Eqs. (2)(3)) were fitted (Table 3) using the RETC software (van Genuchten et al., 1991), based on the measured data. The soil hydraulic properties below 100 cm were taken to be the same as those in the layer immediately above. Since the groundwater table in the experiment was frequently measured and ranged from 86 to 173 cm below the surface, the simulated soil depth was considered to be the distance from the surface to the groundwater table and the soil water content at the lower boundary was set at saturation (Yang et al., 2009).

The crop parameters concerning root growth and root length distribution down the profile were set as follows (see Yang et al., 2009): the root penetration rate K_{rz} of 0.0007 m d^{-1} $^{o}C^{-1}$, the shape parameter controlling root distribution a_z of 3.0, the threshold day temperature for root growth T_{base} of 7 ^{o}C, the temperature for the maximum root growth T_{rmax} of 27 ^{o}C. The parameter values used for estimating potential soil evaporation and crop transpiration were according to the FAO dual crop coefficient approach proposed by Allen et al. (1998). The small time step for calculating evaporation, root water uptake and soil water redistribution was 0.001 d (Yang et al., 2009). The weather information used in the simulation periods, including daily air temperatures, rainfall and global radiation, was measured and given in Groot and Verberne (1991). The date of the first measurement of soil water was used as the starting point in the simulations and set the measured soil water distributions down the profile as the initial conditions.

4.2 HRI experiments for the validation of the updated model

The second part of the study compares the predictions of the updated SMCR_N model against data from the field experiments. Daily measurements of weather variables were made at the on-site weather station. Soil hydraulic properties at various depths are shown in Table 4 (after Fernández-Gálves and Simmonds, 2006). Table 5 lists the parameter values related to crop N-nutritional characteristics, root development, and staged potential evapotranspiration of 4 different species. Such a parameterization over a wide range of crops is given in Zhang et al. (2009). The measured soil mineral N in the top 30 cm was 28.5 kg N ha^{-1} for lettuce, 10.3 kg N ha^{-1} for radish, and 17.8 kg N ha^{-1} for cabbage and soyabean. Soil mineral N in 30-60 cm layer and 60-90 cm were estimated as 10 and 5 kg N ha^{-1}, respectively (Zhang et al., 2007). The model was run from 5 December 2005 when the pre-planting soil sampling was carried out for lettuce and radish. At this time, the initial soil water deficit then was assumed to be zero, i.e the soil water content in the profile was at field capacity. The simulated amounts of soil mineral N were updated for cabbage and soyabean on 6 February 2006 when soil mineral N was measured on these plots. The minimum soil mineral N level c_{Nmin} below which plants are not able to take up N was set 0.0035 kg m^{-3} for all crops (Zhang et al., 2009). Soyabean was different from other crops in that it fixed atmospheric-N to meet crop critical %N form maximum growth when N supply from the soil was limited. The temperature-independent organic matter breakdown rate k_{min} was 0.00015 g g^{-1} d^{-1} (Zhang et al., 2009), in agreement with that used in other models for similar soils (Mueller et al., 1996; Fang et al., 2005). The measured organic carbon contents were 0.8% for lettuce, 0.5% for cabbage, 0.6% for radish and 0.9% for soyabean, respectively. The variation in organic carbon content might be due to the incorporation of different previous crop residues and roots. A value of 3 was used for Q_{10}, a factor for correcting rates of organic matter breakdown for differences in temperature (Hansen et al., 1990). The temperature at which the response function for soil temperature on N mineralization equals 1 was set 20 ^{o}C (Hansen et al., 1990). It was also assumed that soil N mineralization was restricted to the upper 30cm depth of soil.

5. Results and discussion

5.1. Numerical experiment

Fig. 2 compares the soil water content profiles at various time intervals simulated with different approaches. The profiles predicted by the updated SMCR_N model agree well with those from the Richards' equation solved with the FE method. Over the simulation period of 30 days, the maximum error of the proposed approach did not exceed 1% for the coarse soil compared to the FE solution, whereas the maximum error for the fine soil did not exceed 0.8%. However, soil water profiles simulated using the cascade approach in the original SMCR_N model were markedly different from those obtained by the FE method throughout both the soil profile and the simulation period. This is particularly true for the coarse soil (Fig. 2a). The maximum error occurred deeper in the soil column at the early stages of simulation, and then moved up to the surface with increasing time. For example, at t = 24 h the profile computed by the cascade model under-predicted the soil water content at the bottom of the column compared to the FE solution by 28.7% for the coarse soil and by 3.5% for the fine soil. At t = 3 and 9 d, the maximum error increased to 32.3% and 33.6% for the coarse soil, respectively. Likewise, the relative differences were 4.7% and 11% for the fine soil. All of the maximum errors moved up to the surface of the soil columns over time. Since soil water content in the near-surface regions of soil are an important determinant of moisture and energy fluxes to the atmosphere (Shao and Henderson-Sellers, 1996; Lee and Abriola, 1999), incorrect simulation of soil water content in this region inevitably affects the estimates of evaporation and vegetation transpiration.

Fig. 3 compares the total water in the soil column during the simulation period by the different approaches. Again the simulated results from the updated model are in excellent agreement with those from the FE method. In both cases, the maximum error in the whole simulation period was no greater than 1%. In contrast, the results from the cascade model deviated from the FE solution significantly, especially for the coarse soil. At t = 24 h, the cascade model over-predicted drainage from the soil column by 23.3% for the coarse soil, compared with the FE solution. The relative error for the rest of simulation period ranged from 16% to 29%. For the fine soil, the performance of the cascade model was satisfactory in predicting drainage, with the maximum relative error all within 3%. This can be attributed to the slow water flow in this soil. The computed water fluxes at the lower boundary are similar for all the methods, but the distributions of water contents are noticeably different in the near-surface region (Fig. 2).

5.2. PGAV experiment

To evaluate the overall model performance in predicting soil water dynamics in the soil-crop system where all the processes governing water transfer from soil to the atmosphere were considered, all the measurements of soil water content from the experiment in different soil layers at time intervals were compared with the simulations by the updated and the original models (Fig. 4). Regressions of simulated and measured gave a similar R^2 value for both models, which suggests that both the original and the updated models were all able to simulate the change patterns in soil water content. However, the gradient of approximately to 1 and the intercept of approximately to 0.0 from the updated model show that the simulated values of soil water content from the updated model agreed much better with the measured values (all the data points are close to the 1:1 line) than those from the original model.

Soil water contents in 20 cm layers to 1 m were compared between the measured and the simulated using the updated and the original models in detail over time (Fig. 5). It can be observed that the updated model not only reproduced the patterns of soil water changes in layers, but also produced values close to the measurements. However, the original model severely under-estimated soil water content in the layers of 20-40 cm and 40-60 cm, especially at the late crop development stages. The marked discrepancies between measurement and simulation by the original model can be attributed to the inability of the model to simulate capillary flow caused by the relatively high groundwater table in the experiment.

From the above, it is evident that the updated model performed much better than the original model in simulating soil water dynamics and water drainage in the soil-crop system. The updated SMCR_N model produced nearly the same results as these by the FE approach which is highly accurate but complex in implementing the numerical scheme in predicting water drainage in the soil, and reproduced well the spatial-temporal soil water content in the PAGV field experiment. This confirms the findings from the previous studies (Gandolfi et al., 2006; Cannavo et al., 2008) that the cascade algorithm for hydrological simulation produces poor results and requires improvements to make better predictions. The update of the model using the simple procedure for solving the basic flow equation (Yang et al., 2009) has proven to be a success for improving predictions and, more importantly, for extending the model application to the circumstances such as where the capillary flow is important as demonstrated in the study.

5.3. Validation experiments

In the validation of the updated SMCR_N model against data from the experiments on 4 crops, we focused our attention on processes in the plant and in the soil in the top 90 cm, although the soil domain was calculated to 2 m in depth. The primary reason for this was for most crops 90% of their roots are located in the top 90 cm soil (Burns, 1980; Greenwood et al., 1982). There is little chance of crops recovering mineral-N leached below 90 cm from the surface and any such N is considered to be a potential source of groundwater pollution.

N offtake by the plant (excluding fibrous roots at harvest) and mineral N in the top 90 cm of soil for the 4 crops were simulated and compared with the measured values. Fig. 6 shows that the simulated data are not only highly correlated to, but also almost proportional to the corresponding measured values for all crops. During the simulations, no parameter values were adjusted to improve the fit between measurement and simulation. This suggests that the model is properly constructed and well parameterized for the tested conditions and is, therefore, able to make reasonable predictions for the response of crop to N fertilizer, and N losses from the root zone by leaching.

N dynamics in the different experiments was simulated and shown for the soyabean experiment (see Fig. 7). The variation of N mineralization from soil organic matter followed a similar pattern to the changes in air temperature, with the maximum N mineralization occurring in summer (Fig. 7a). The simulated N mineralization rate was 0.6 kg ha^{-1} d^{-1} at 20^{o}C, close to the value of 0.7 kg ha^{-1} d^{-1} at 16^{o}C derived from the measurements on the same soil (Greenwood and Draycott, 1989). N offtake by the crop increased with time in the early stages of growth, but decreased towards maturity. This is a result of the dual action of a lower crop %N required for maximum growth and a reduction in growth rate caused by lower temperatures in the later growth stages (Fig. 7b). Soyabean is a crop capable of atmosphere-N fixation. When N supply from the soil is limited, the crop fixes atmosphere-N to meet critical %N for the maximum growth. Atmosphere-N fixation occurred only when the mineral N in the soil was depleted to a minimum level below which no N uptake was possible, and thus started at a later date than planting (Fig. 7b). A total of 148 out of the 205 kg-N ha^{-1} recovered by this crop was fixed during the course of the experiment. Temporal mineral N in the top 90 cm soil for different crops is plotted in Fig. 8. The sudden increases in soil mineral N were due to the application of fertilizer-N, while the more gradual increases were attributed to N mineralization from soil organic matter. The sharp decreases in soil mineral N were the result of N uptake by crops. Since there was no fertilizer-N applied to the soyabean crop, the mineral N in the top 90 cm soil was general lower than those in other experiments.

All crops suffered from water stress to varying degrees as the accumulated actual transpirations were less than the potential ones (Fig. 9). Radish suffered from water stress most severely, whereas lettuce suffered the least. One contributory factor to the high water stress of radish is that the crop was planted in the summer, when rainfall was very sparse. The crop only grew for 27 days, and in the first 22 days the crop lost a total of about 82.5 mm water by evapotranpiration. However, the water infiltration in the same period was only 20 mm. Furthermore, radish is a shallow-rooted crop, which makes it less able to extract water from depth in the soil profile. Compared with the other crops cabbage is a relatively deep-rooted species with a fairly even root distribution (Thorup-Kristensen, 2006). This means the crop is able to extract water from a bigger soil volume. Nevertheless, the total demand for evapotranspiration during growth of cabbage of 491 mm was much greater than the total water infiltration of 220 mm, resulting in shortage of soil water for the crop to take up. This evidence suggests that the model is able to simulate water uptake sensibly for various crop species.

Leaching mainly occurred in winter when rainfall was high and evaporative demand was small, as demonstrated in the soyabean experiment (Fig. 10). No significant leaching occurred during the summer when evapotranspirative demand was high. This is supported by previous studies which showed that most leaching occurs between late autumn and early spring, when the soil is not covered by crops in European conditions (Neeteson and Carton, 2001). Since N leaching and water percolation are coupled processes, the cumulative N leaching curves (Fig. 11b) have the same trends as those in water losses (Fig. 11a). In both lettuce and radish experiments, water percolation below 90 cm was greater, resulting from the relatively short growth periods of these crops. This, together with higher mineral N concentrations present in the soil (Fig. 8), led to greater N losses by leaching. The cumulative N leaching in the lettuce and radish experiments was approximately 20 kg-N ha^{-1} by the end of simulations, about three times higher than that in the cabbage and soyabean experiments.

5.4. Model evaluation

The improvement of modeling water dynamics in the soil-crop system has been clearly demonstrated in reproducing the results from the PAGV experiment. The predicted spatial-temporal soil water content using the updated model was in good agreement with the measurements, whereas the original model could not satisfactorily reproduce results in the deep soil where water content was greatly affected by groundwater table. By employing the recently developed numerical scheme for the basic soil water flow equation (Yang et al., 2009) in the updated model, the model not only produced the identical results as those from the complex FE numerical scheme in simulating the internal water drainage in different soils (Fig. 2), but also allowed us to model capillary flow caused by high groundwater table, which has led to the extension of the model application.

It is difficult to rigorously assess the performance of any crop N model on N dynamics since N transfer in some processes such as N incorporation in roots is hard to measure precisely. In this study it is even more difficult to do so because soil mineral N was not frequently monitored in the experiments. However, some assessment of the performance of the model on N dynamics is still possible based on the following lines of evidence: 1) both the simulated values of N uptake in the above-ground dry weight in all the experiments and the mineral N in 90cm soil depth on the measured dates were close to the measured values; 2) although the simulated N incorporated in the roots could not be quantitatively validated because the experimental data was unavailable, the approach for considering N partitioned in roots has previously been proved acceptable for many crops (Zhang et al., 2009); 3) the soil organic matter breakdown rate used was similar to those used in other models (Mueller et al., 1996; Fang et al., 2005), and the simulated N mineralization rate of 0.6 kg ha^{-1} d^{-1} at 20^{o}C was close to the value of 0.7 kg ha^{-1} d^{-1} at 16^{o}C derived from the measurements on the same soil (Greenwood and Draycott, 1989); 4) the simulated N leaching from 90 cm soil depth was small during early spring and late autumn, which was supported by the finding of Neeteson and Carton (2001); 5) N losses from the processes such as ammonia volatilization and denitrification were not simulated, but were previously found to be small in this sandy loam soil (Zhang et al., 2007, 2009).

Thus, it is reasonable to conclude that the updated model performed well in predicting water and N dynamics in the soil-crop system for the cases studied. There is a need though to extend the functions of the model to simulate soil processes such as denitrification, ammonia volatilization and ammonia fixation to further widen its application.

6. Conclusions

A generic agro-hydrological model SMCR_N for the effect of N fertilizer on crop growth and nitrate leaching has crucially been updated by replacing the existing approximate hydrological algorithms with a simple and accurate approach based on the basic flow equation. The updated model strikes a balance between accuracy, simplicity and robustness. The model not only consistently out-performs the original model in predicting internal water drainage in different soils and water dynamics in the complex soil-wheat system, but also extends its use to the situations where the capillary flow is important. Due to the highly accurate algorithm for hydrological simulation, the updated model can now be employed for rigorous study of water dynamics in the soil-crop system as well.

Validation of the updated SMCR_N model against data from field experiments on 4 contrasting crops shows that the model is capable of reproducing the measured data. The simulated results agree well with the measured values, indicating that the updated SMCR_N model has been properly devised and parameterized. This, and its validation against the comprehensive datasets of water and N measured in the wheat experiments (Zhang, 2010) and the validation of the original model on 16 vegetable crops (Zhang et al., 2009), provides the model with the potential to optimize water and N use and assess the impact of N leaching from different management strategies in crop production where diverse crops are grown.

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Figure captions:

Fig. 1. Schematic representation of the model. The algorithms in the grey box are implemented using a small time step 0.001d, while the other processes are simulated using a time step of 1 d.

Fig. 2. Soil water content distributions simulated using different approaches for a coarse soil (a) and a very fine soil (b) draining from saturation after 1d, 3d and 9d. Solid line represents the simulated results from the updated SMCR_N model. Symbols open triangle and square represent the results from a finite element (FE) method and the original SMCR_N model, respectively.

Fig. 3. Variation of the total water in a 200cm soil column with time calculated using different approaches for a coarse soil (a) and a very fine soil (b) draining from saturation. Solid line represents the simulated results from the updated SMCR_N model. Symbols open triangle and square represent the results from a finite element (FE) method and the original SMCR_N model, respectively.

Fig. 4. Overall comparison of soil water content down the profile at time intervals between measurement and simulation using the original model and the updated model in the PAGV experiment. Symbols open triangle and open square represent the results from the original and updated models, respectively.

Fig. 5. Comparisons of soil water content θ in relation to the time DOY (day of the year) between measurement and simulation using the updated and the original

models in the layers of 0 – 20 cm (a), 20 – 40 cm (b), 40 – 60 cm (c), 60 – 80 cm (d), and 80 – 100 cm (e) in the PAGV experiment. Solid and dotted lines represent the simulations by the updated and original models, respectively. Symbol open triangle represents the measurement.

Fig. 6. Comparisons between the measured and simulated N offtake in the plants excluding fibrous roots (a) and mineral N in 90cm soil (b) for different crops. The vertical bars represent the ranges of the measured values.

Fig. 7. Simulated daily N mineralization from soil organic matter (a) and N offtake and N fixation (b) in the soyabean experiment.

Fig. 8. Simulated temporal changes in soil mineral N in the top 90 cm in different experiments.

Fig. 9. Simulated cumulative potential (T_{pot}) and actual (T_{act}) transpiration for cabbage and soybean (a), and lettuce and radish (b).

Fig. 10. Simulated daily water percolation and N leaching at 90 cm depth in the soyabean experiment.

Fig. 11. Simulated cumulative water percolation (a) and N leaching (b) at 90 cm depth in different experiments.

Table 1
Experimental details

Crop	Spacing (cm)	Sowing date	Transplanting date	Harvest date	Water volume (mm) and date of irrigation			N fertiliser rate (kg N ha^{-1}) and date of fertilisation		Dry matter yield (t ha^{-1})
Lettuce	20 x 20	-	11/08/06	09/10/06	5 (18/08/06)	-	-	100 (10/04/06)	-	4.03
Cabbage	20 x 35	-	16/05/06	07/09/06	10 (04/07/06)	5 (14/07/06)	10 (20/07/06)	100 (12/05/06)	200 (20/06/06)	8.11
Radish	30 x 4	18/08/06	-	14/09/06	5 (18/08/06)	-	-	100 (10/04/06)		1.86
Soyabean	7 x 3	11/07/06	-	17/10/06	5 (20/07/06)	-	-	-	-	5.80

Table 2
Soil hydraulic properties used in the numerical experiments (θ_s, θ_r, α, n are the van Genuchten soil hydraulic property parameters, representing the saturated and residual soil water content, the shape parameters of the retention and conductivity functions. K_s and θ_{FC} are the saturated hydraulic conductivity and the soil water content at field capacity, respectively)

Soil type	θ_S (cm^3 cm^{-3})	θ_r (cm^3 cm^{-3})	α (cm^{-1})	n	K_s (cm d^{-1})	θ_{FC} (cm^3 cm^{-3})
Coarse soil	0.40	0.03	0.0383	1.377	60.0	0.17
Very fine soil	0.61	0.01	0.0265	1.103	15.0	0.49

Table 3
Fitted soil hydraulic properties in the PAGV experiment using the RETC software (van Genuchten et al., 1991) (See Table 2 for the meanings of the symbols in the Table)

Soil depth (cm)	θ_s ($cm^3\ cm^{-3}$)	θ_r ($cm^3\ cm^{-3}$)	α (cm^{-1})	n	K_s ($cm\ d^{-1}$)
0–25	0.42	0.04	0.0162	1.299	160.0
25–40	0.50	0.06	0.0096	1.346	33.0
40–100	0.53	0.06	0.0098	1.319	200.0

Table 4
Soil hydraulic properties in the soil profile in the validation experiments (See Table 2 for the meanings of the symbols in the Table)

Soil depth (cm)	θ_s (cm^3 cm^{-3})	θ_r (cm^3 cm^{-3})	α (cm^{-1})	n	K_s (cm d^{-1})
0 – 25	0.37	0.04	0.0042	1.178	28.0
25 – 45	0.35	0.05	0.0214	1.119	34.0
45 – 200	0.38	0.06	0.0267	1.341	18.0

Table 5
Crop parameter values related to the maximum %N in the main (shoot and tap root) and root compartments, root development and transpiration

CROP	N fixation	α_N[a]	β_N[a]	R_{lux}[a]	Root penetration rate (m d^{-1} $^{o}C^{-1}$)	a_z[b]	Crop coefficient for potential transpiration			Length of growth stage (d)			
							initial	middle	end	initial	development	middle	late
Cabbage	No	3.45	0.6	1.0	0.0014	1.5	0.15	0.95	0.85	40	60	50	15
Lettuce	No	2.6	1.1	1.0	0.001	2	0.15	0.9	0.9	30	40	25	10
Radish	No	1.35	1.87	1.2	0.001	3	0.15	0.85	0.75	5	10	15	5
Soyabean	Yes	1.37	1.7	1.0	0.001	3	0.15	1	0.7	20	30	70	20

[a] crop N nutrition coefficients in Eqs. (9), (10) and (15).
[b] shape parameter for root length distribution down the soil profile in Eq. (12).

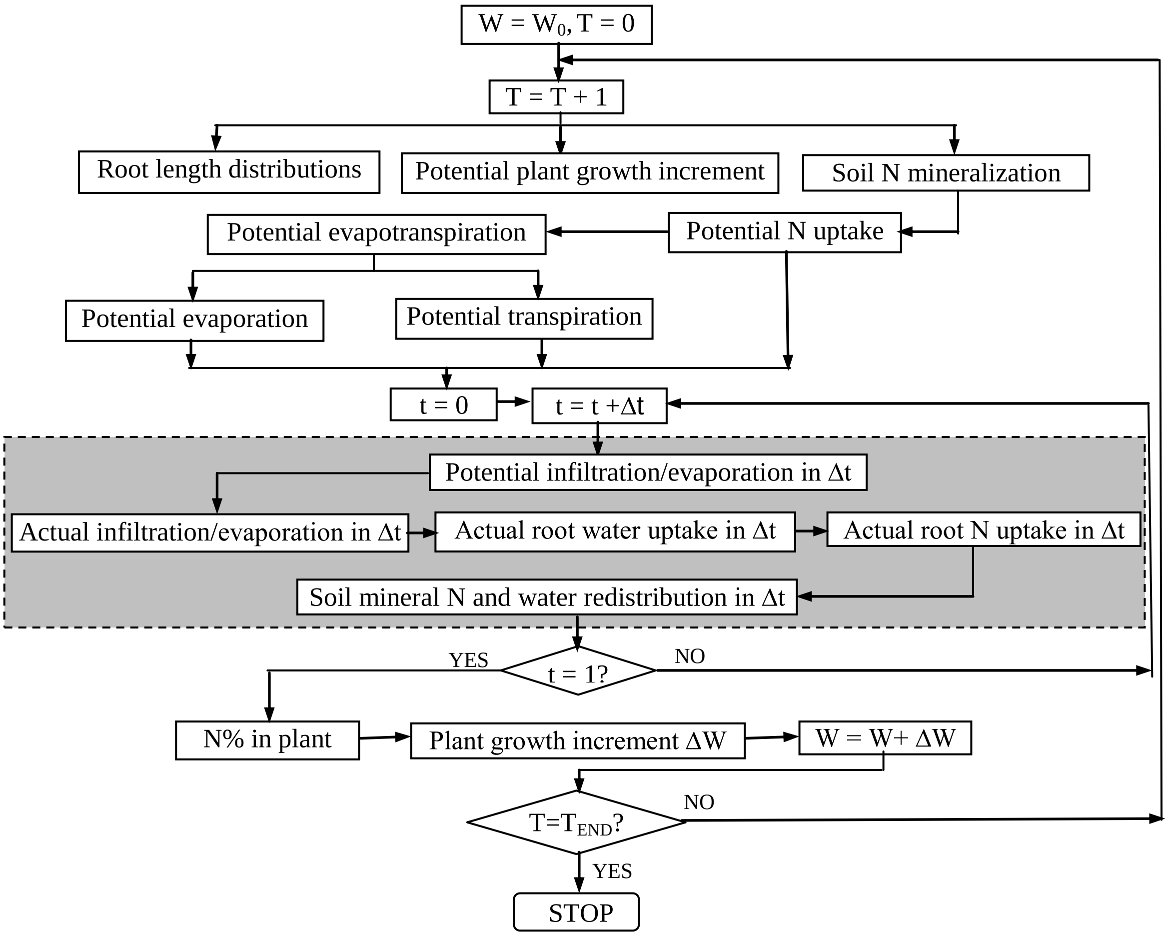
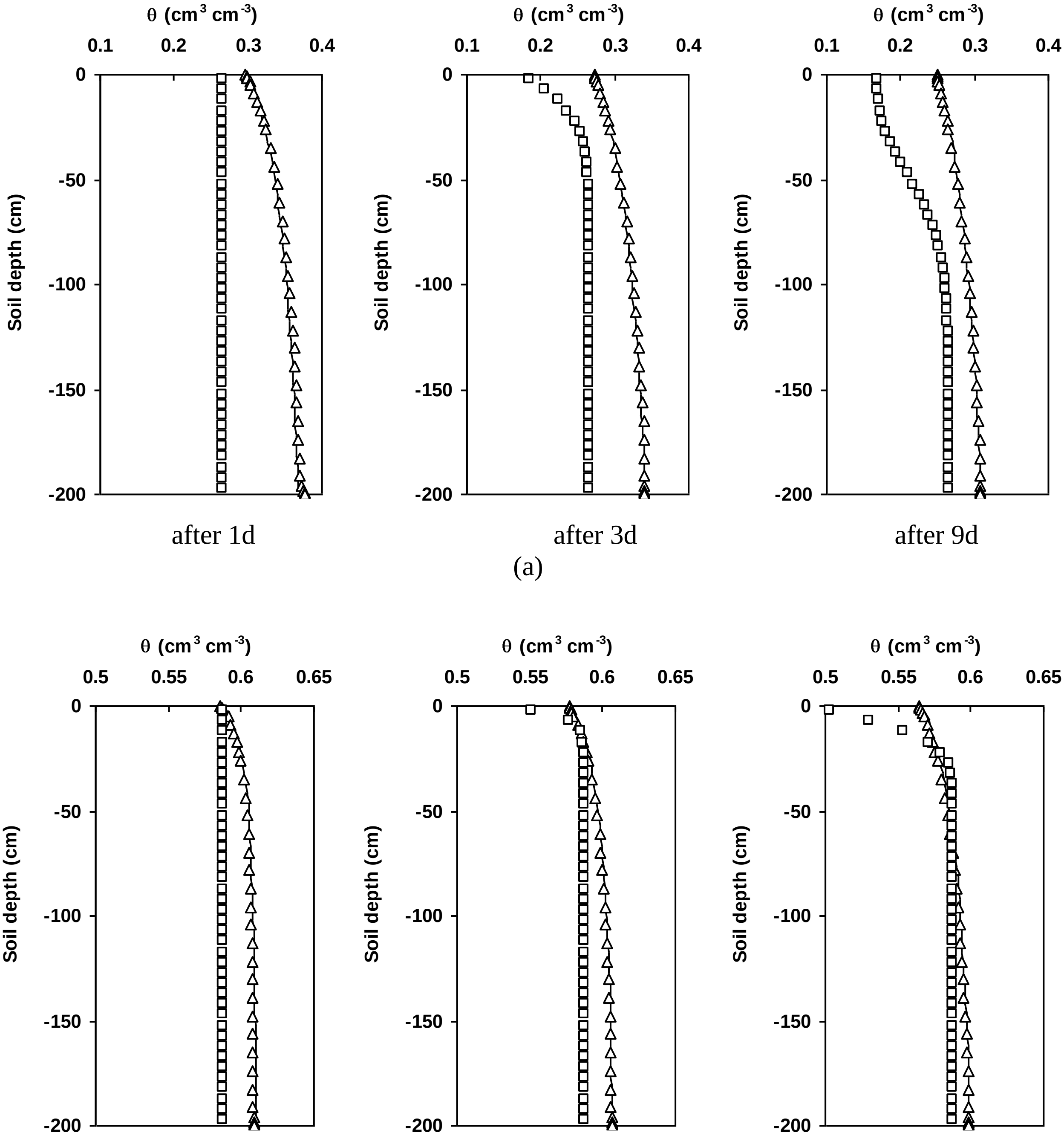

W = W0, T = 0
T = T + 1
Root length distributions
Potential plant growth increment
Soil N mineralization
Potential evapotranspiration
Potential N uptake
Potential evaporation
Potential transpiration
t = 0
t = t +Δt
Potential infiltration/evaporation in Δt
Actual infiltration/evaporation in Δt
Actual root water uptake in Δt
Actual root N uptake in Δt
Soil mineral N and water redistribution in Δt
YES
t = 1?
NO
N% in plant
Plant growth increment ΔW
W = W+ ΔW
NO
T=TEND?
YES
STOP

Fig.1



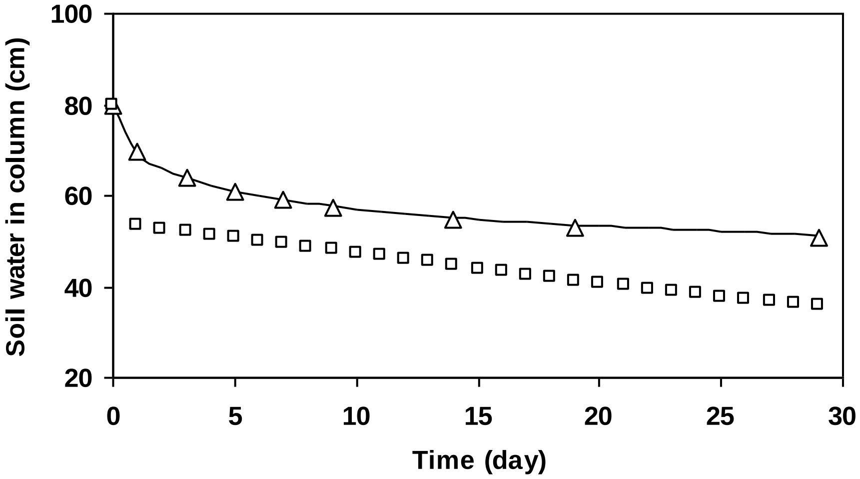
after 1d after 3d after 9d

(a)

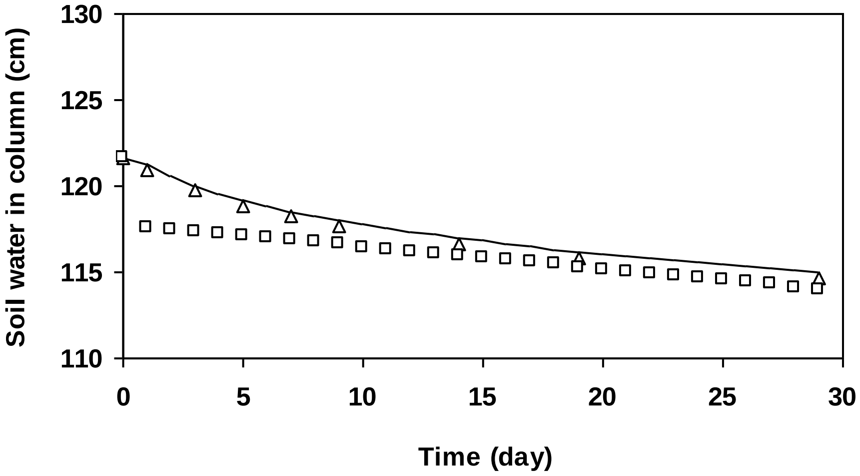
after 1d after 3d after 9d

(b)

Fig. 2


100
80
60
40
20
Soil water in column (cm)
0
5
10
15
20
25
30
Time (day)

(a)


130
125
120
115
110
Soil water in column (cm)
0
5
10
15
20
25
30
Time (day)

(b)

Fig. 3

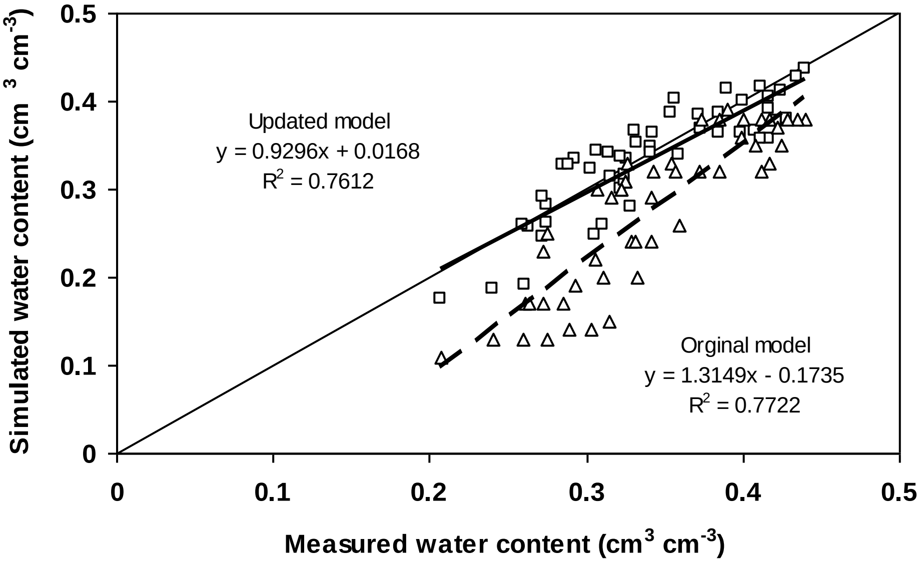

Simulated water content (cm 3 cm-3)
0.5
0.4
0.3
0.2
0.1
0
Updated model
y = 0.9296x + 0.0168
R2 = 0.7612
Orginal model
y = 1.3149x - 0.1735
R2 = 0.7722
0
0.1
0.2
0.3
0.4
0.5
Measured water content (cm3 cm-3)

Fig. 4

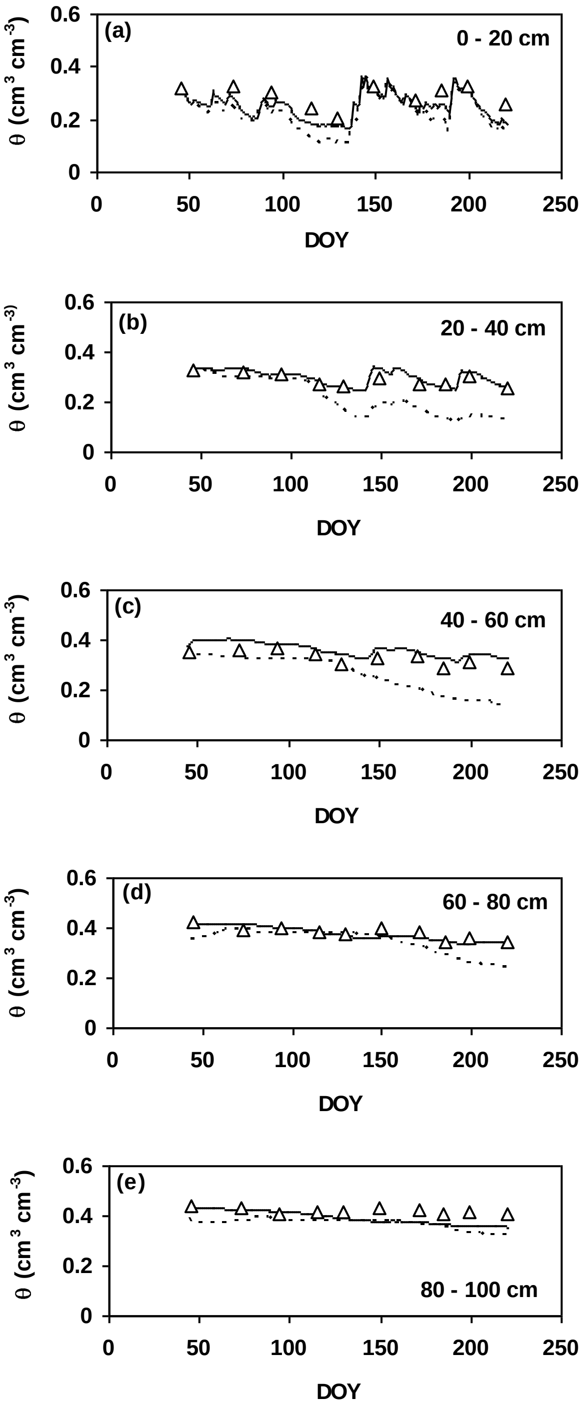
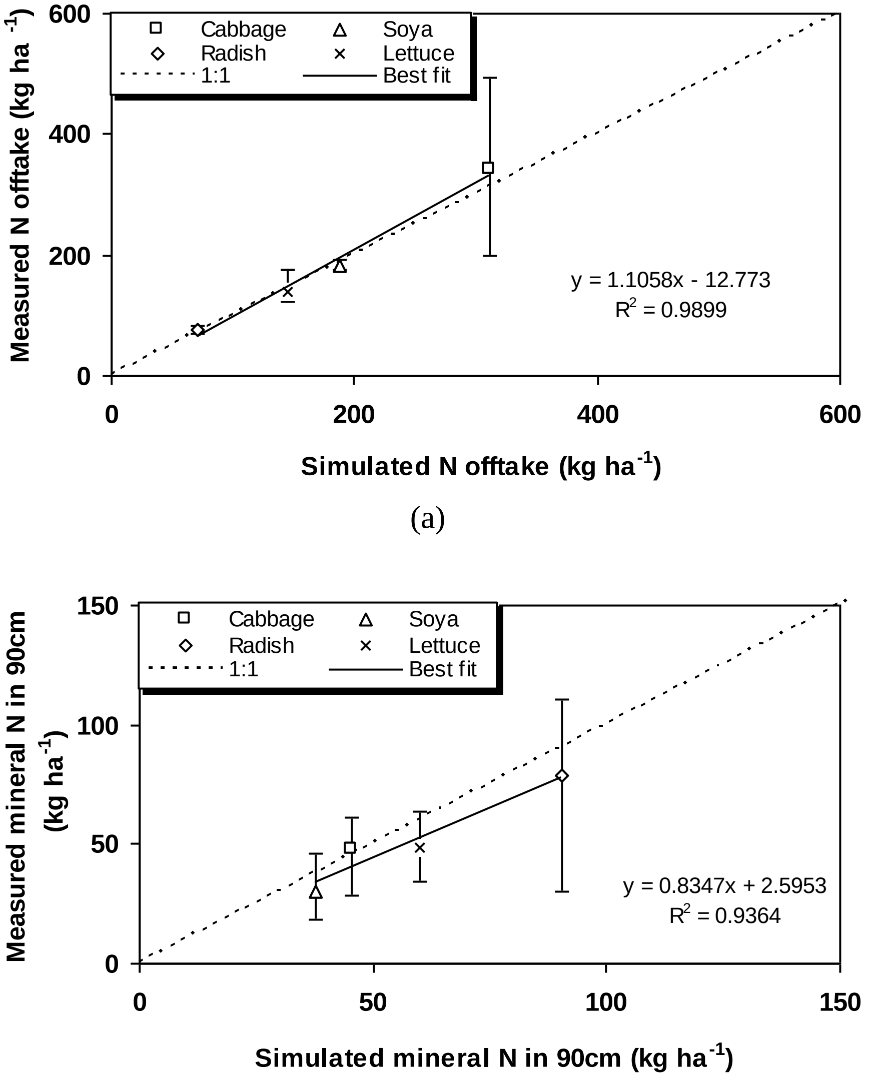

(a)
0 - 20 cm
(b)
20 - 40 cm
(c)
40 - 60 cm
(d)
60 - 80 cm
(e)
80 - 100 cm
θ (cm3 cm-3)
0
0.2
0.4
0.6
0
50
100
150
200
250
DOY

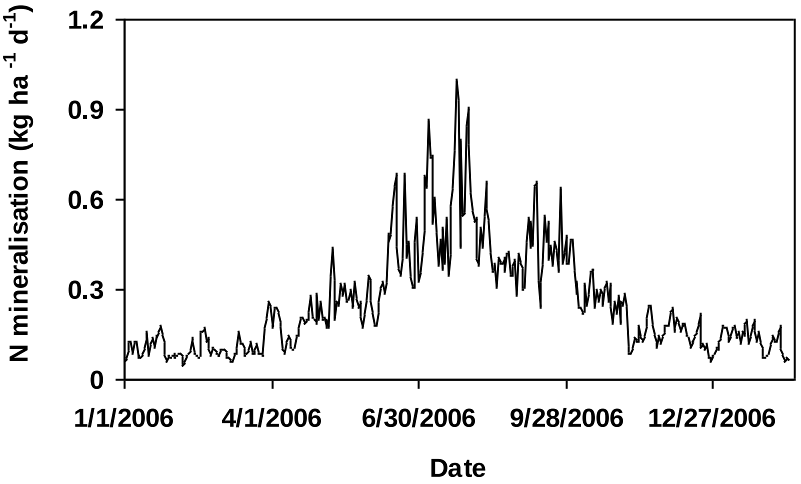
Fig. 5


Cabbage
Soya
Radish
Lettuce
1:1
Best fit
Measured N offtake (kg ha $^{-1}$)
600
400
200
0
0
200
400
600
Simulated N offtake (kg ha^{-1})
y = 1.1058x - 12.773
R^2 = 0.9899
Cabbage
Soya
Radish
Lettuce
1:1
Best fit
Measured mineral N in 90cm (kg ha^{-1})
150
100
50
0
0
50
100
150
Simulated mineral N in 90cm (kg ha^{-1})
y = 0.8347x + 2.5953
R^2 = 0.9364

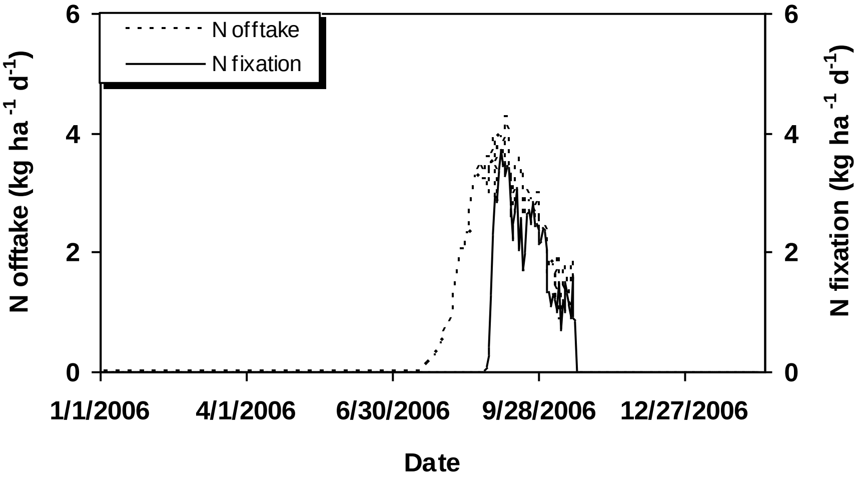
(a)

(b)

Fig. 6


N mineralisation (kg ha $^{-1}$ d^{-1})
1.2
0.9
0.6
0.3
0
1/1/2006
4/1/2006
6/30/2006
9/28/2006
12/27/2006
Date

(a)


N offtake
N fixation
N offtake (kg ha $^{-1}$ d^{-1})
N fixation (kg ha $^{-1}$ d^{-1})
6
4
2
0
1/1/2006
4/1/2006
6/30/2006
9/28/2006
12/27/2006
Date

(b)

Fig. 7

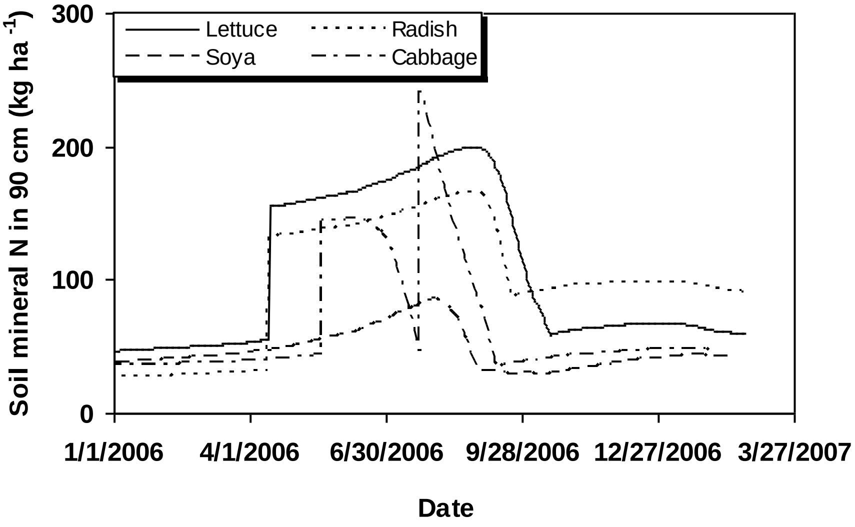
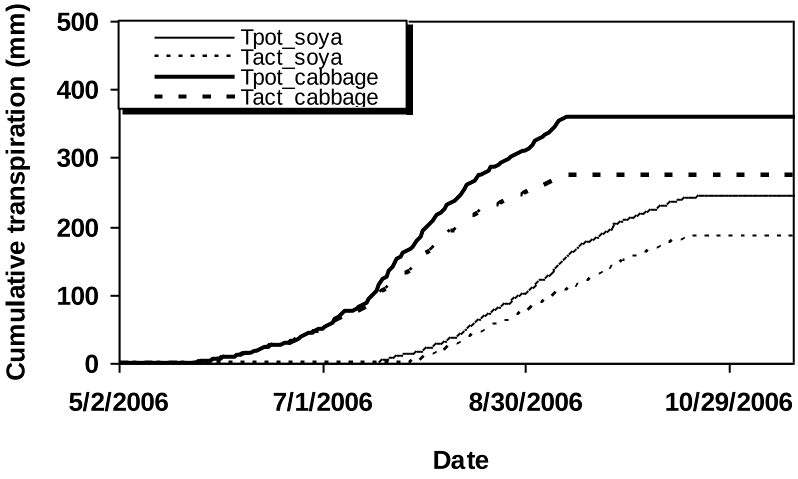
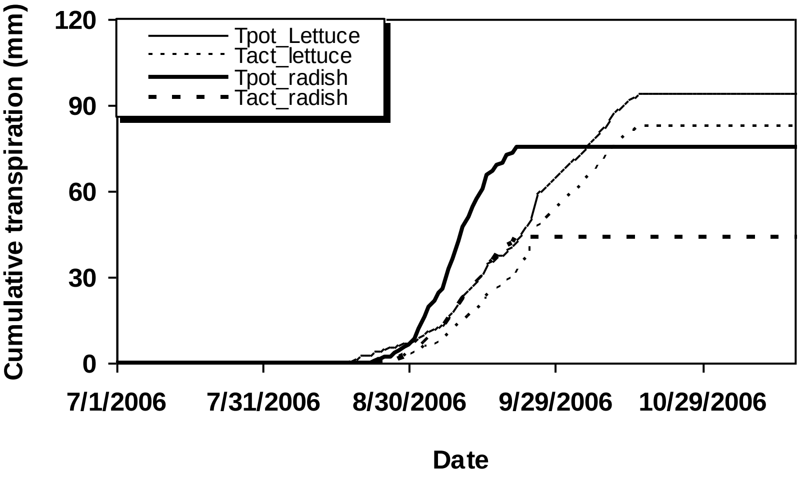

Lettuce
Radish
Soya
Cabbage
Soil mineral N in 90 cm (kg ha -1)
300
200
100
0
1/1/2006
4/1/2006
6/30/2006
9/28/2006
12/27/2006
3/27/2007
Date

Fig. 8


Cumulative transpiration (mm)
500
400
300
200
100
0
Tpot_soya
Tact_soya
Tpot_cabbage
Tact_cabbage
5/2/2006
7/1/2006
8/30/2006
10/29/2006
Date

(a)


Cumulative transpiration (mm)
120
90
60
30
0
Tpot_Lettuce
Tact_lettuce
Tpot_radish
Tact_radish
7/1/2006
7/31/2006
8/30/2006
9/29/2006
10/29/2006
Date

(b)

Fig. 9

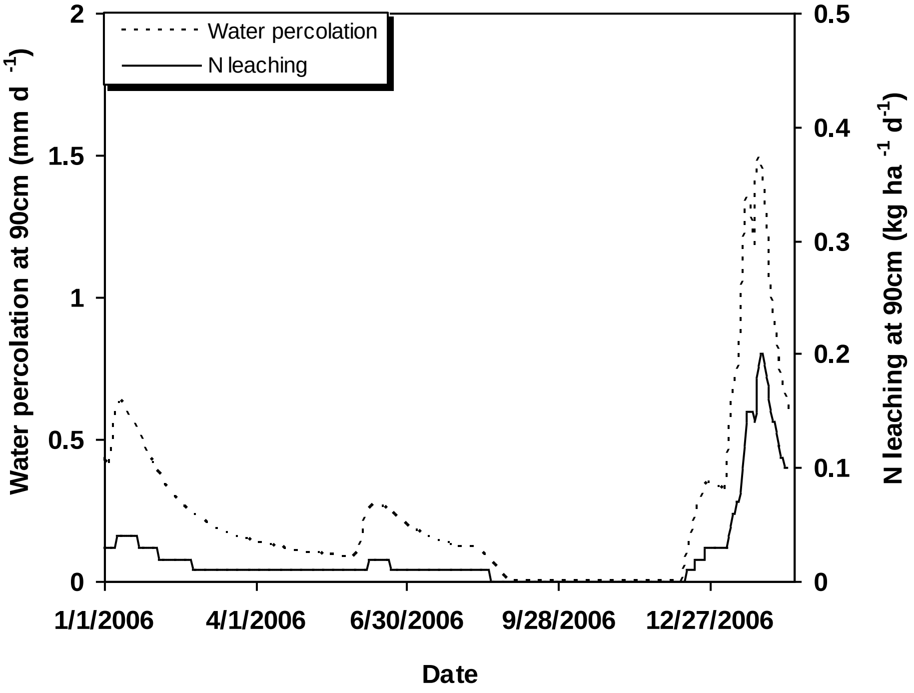
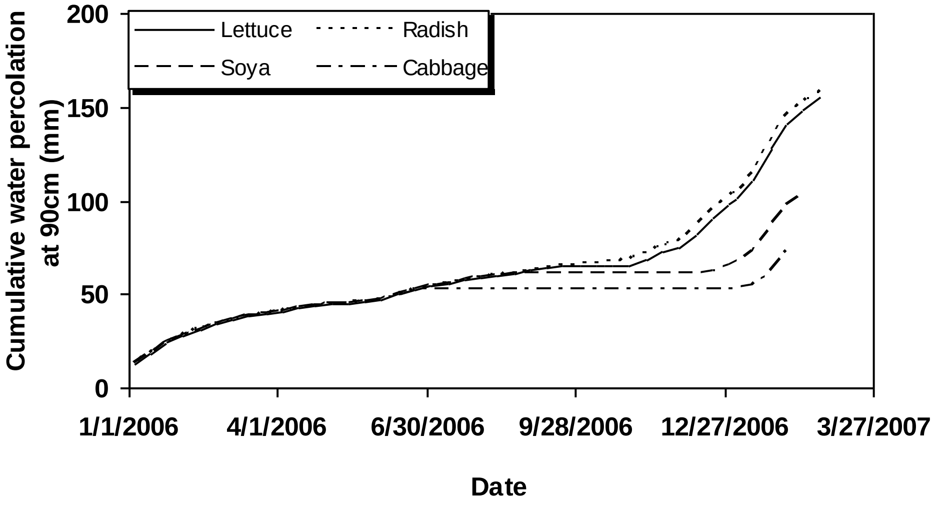
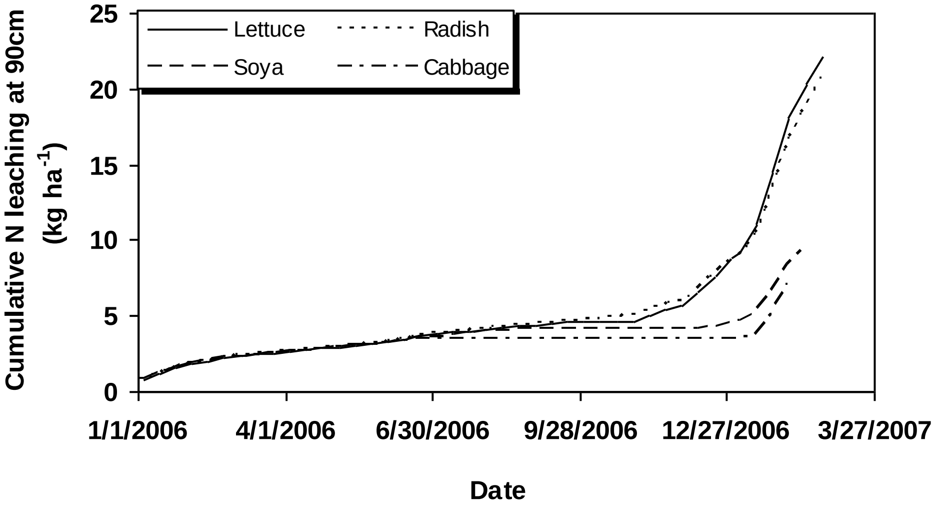

Water percolation
N leaching
Water percolation at 90cm (mm d $^{-1}$)
N leaching at 90cm (kg ha $^{-1}$ d^{-1})
2
1.5
1
0.5
0
0.5
0.4
0.3
0.2
0.1
0
1/1/2006
4/1/2006
6/30/2006
9/28/2006
12/27/2006
Date

Fig. 10


200
150
100
50
0
Cumulative water percolation at 90cm (mm)
1/1/2006
4/1/2006
6/30/2006
9/28/2006
12/27/2006
3/27/2007
Date
Lettuce
Radish
Soya
Cabbage

(a)


25
20
15
10
5
0
Cumulative N leaching at 90cm (kg ha^{-1})
1/1/2006
4/1/2006
6/30/2006
9/28/2006
12/27/2006
3/27/2007
Date
Lettuce
Radish
Soya
Cabbage

(b)

Fig. 11