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An explicit hydrological algorithm for basic flow and transport equations and its application in agro-hydrological models for water and nitrogen dynamics

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Abstract

Hydrological simulation is a key component in argo-hydrological models for optimizing resources use and minimizing the environmental consequences in agriculture. In this study we extended a simple and explicit algorithm for solving the basic soil water flow equation by Yang et al. (J. Hydrol. 370, 177-190) to the solute transport equation. The key feature of the algorithm is to use a uniform soil layer thickness and a small time step in solving the soil water and solute transport equations, so that the calculations can be made on a layer basis. This drastically simplifies the procedure of modeling water and solute transport in soil using the basic equations. The proposed algorithm was tested against the complex finite element (FE) numerical scheme in simulating soil water and solute transport in different soils via numerical experiments. The results showed that the proposed algorithm with a uniform soil layer thickness of 5 cm and a small time step of 0.001d was able to achieve the identical accuracy as the FE method. Tests of the proposed algorithm in simulating water and nitrogen dynamics against data from a field experiment on wheat revealed that the predicted results with the simple algorithm were in good agreement with the time-course measurements of soil water and mineral N concentration at the various depths in the profile, suggesting that the proposed algorithm performed well and can be reliably applied in agro-hydrological models. The simplicity and accuracy of the algorithm will encourage scientists to use basic equations for soil water and solute transport more in the future for improving performance of agro-hydrological models.

Key words: Richards' equation, transport equation, soil-crop system, soil water movement, solute transport.

1. Introduction

With the advance in computing power and increasingly understanding of soil and plant sciences, process-based agro-hydrological models have become powerful tools in optimizing resources use and minimizing environmental consequences in crop production. Numerous agro-hydrological models have been devised for the optimal use of water, fertilizer and pesticide in the literature over the last few decades (see reviews by Bastiaanssen et al.; 2007; Cannavo et al., 2008; Ranatunga et al., 2008). For example, according to the review by Cannavo et al. (2008), for crop nitrogen (N) models alone, there are 62 models available for evaluating the effect of different N management on plant growth and environmental impacts.

Hydrological simulation is a key module in agro-hydrological models. Mainly there are two approaches used for hydrological simulations in such models, i.e. cascade approach and numerical method based on basic soil water flow and solute transport equations (Bastiaanssen et al., 2007; Cannavo et al., 2008; Ranatunga et al., 2008). The cascade approach assumes that water moves into the soil profile where it is routed through the soil layers, and the solute transports with water flow. Water drains between two soil layers when the soil water is above field capacity. Due to the simplicity of the algorithm and stability of numerical results, the cascade approach has been used in many agro-hydrological models for hydrological simulations (Arnold et al., 1993; Ritchie, 1998; Greenwood, 2001; Droogers et al., 2001; Brisson et al., 2003; Zhang et al., 2007, 2009; Renaud et al., 2008; Pederson et al., 2009; Raes et al., 2009). Cannavo et al. (2008) surveyed 16 models for predicting nitrate leaching in the cropped soils, and found that a large proportion (7 out of 16) of models adopted this approach. However, as pointed out by Cannavo et al. (2008), this approach cannot correctly simulate soil water content between field capacity and saturation, which has become a severe limitation for calculating denitrification. Further, this approach produces poor daily drainage dynamics, and is not capable of simulating capillary flow (Gandolfi et al., 2006), and thus cannot be applied in the cases where groundwater table is high and capillary flow is important to meet crop evapotranspiration. Besides it is difficult to implement precise boundary conditions, such as free drainage, often imposed at the lower boundary in a cascade approach (Yang et al., 2009), which could result in unacceptable results as the hydrological results are highly sensitive to parameterization at the lower boundary (Boone and Wetzel, 1996).

The other approach, named the numerical method, uses the basic equations for soil water movement and solute transport, and generally produces more accurate results, compared to those by the cascade algorithm (Gandolfi et al., 2006; Yang et al., 2009). Such an approach is now widely accepted, especially in the research models. However, the uptake of models of this type for practical use is still low (Bastiaanssen et al. 2007). One reason for this might be due to the complex nature of the numerical methods involved, and the associated long program code (Yang et al., 2009). Since these equations are highly non-linear partial differential equations, complex numerical schemes, such as finite element (FE) method, are often employed to solve the equations (Šimůnek et al., 1992). This contrasts with the simple algorithms used in modeling other processes such as plant dry matter accumulation, root growth, solute reactions and transformations in agro-hydrological models (Cannavo et al., 2008;

Zhang et al., 2009). Although the numerical schemes such as the FE method used for the solutions to the basic equations are well developed (Šimůnek et al., 2008), and software such as HYDRUS-1D and HYDRUS (2D/3D) (Šimůnek et al., 2005; 2006) is readily available for 1-D or multi-dimensional simulations, its use requires specialized expertise that many potential users have not got. Further, the numerical solutions to the transport equation often exhibit oscillatory behavior, especially when relatively steep concentration fronts are simulated (Šimůnek et al., 1992). Extra measures such as ‘upstream weighting and artificial dispersion coefficients’ are therefore often introduced within the FE method, which makes the numerical scheme even more complex. This partially explains why many agro-hydrological models in practical use, as reported in Cannavo et al. (2008), do not adopt this method for water and nutrients management in agriculture.

Apart from cascade models and numerical methods, attempts have long been made to derive analytical solutions to the basic flow equation (Green and Ampt, 1911; Gardner, 1958; Philip, 1958; Parlange, 1971; Parlange et al., 1985; Mollerup, 2007; Wang et al., 2009). Since the flow equation is a highly non-linear differential equation, assumptions have to be made in deriving such analytical solutions. These assumptions include: soil hydraulic conductivity is an analytical function of soil water content; hysteresis is neglected; and the medium is homogeneous and isotropic (Feddes et al., 1988). Due to these restrictions, together with the difficulties in dealing with the initial soil water distributions and boundary conditions, the derived solutions have found limited application. Although there are reports on the studies of water infiltration into layered soils using the similar approach (Hachum and Alfaro, 1980; Chu and Marino, 2005) and of the development of the kinematic models for soil water movement and solute transport for unsaturated groundwater recharge (Charbeneau, 1984), the derived algorithms are only able to estimate the wetting front in the events of water infiltration, and are not capable of simulating capillary flow and predicting soil water content distribution. Thus they are not appropriate to be employed in agro-hydrological models in which the simulation of upwards water flow resulting from evaporation in layered soils is crucially important.

A new approach using the integrated Richards' equation (IRE) strategy has been proposed and tested for water transfer in the soil-crop system (Yang et al., 2009). The approach, based on the work by Lee and Abriola (1999), strikes a balance between the simplicity and robustness of cascade approaches and accuracy of numerical methods. The IRE approach considers that water content in a soil layer is only influenced by neighbouring layers, i.e. the above and below layers. The water flux between two soil layers is calculated by integrating the Richards' equation over the layer in a small time step. It has been demonstrated that the algorithm worked well with 5 cm layer thickness and a time step of 0.001 d in different cropped soils (Yang et al., 2009). However, the approach is only valid for soil water movement, and therefore cannot be applied in simulating solute transport in the soil which is a key process in agro-hydrological models for fertilizer and pesticide practices.

The objectives of this study were three-folds: 1) to formulate the simple and explicit algorithm using the integration strategy over the basic equations for soil water movement and solute transport by extending the work by Yang et al. (2009), so that the proposed algorithm can have a wide application in agro-hydrological models; 2) to evaluate the proposed algorithm against the FE method in simulating water and solute dynamics in different soils via numerical experiments; 3) to validate the proposed approach in predicting water and N dynamics in a soil-wheat system against data from a field experiment.

2. Theory

2.1 Governing equations for water and solute dynamics in the soil-crop system

In 1-D situations, the differential equations for water and solute transfer within the soil profile in the soil-crop system, based on the general governing equations for water flow and solute transport in porous media (Bear, 1972), are

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

$$\frac{\partial \theta c}{\partial t} = \frac{\partial}{\partial z}(\theta D_z \frac{\partial c}{\partial z}) - v_z \frac{\partial c}{\partial z} + f - S_c \qquad (2)$$

where θ (L^3 L^{-3}) is the volumetric soil water content, h (L) is the soil pressure head, S_w (L^{-1}) is the sink term, i.e. root water uptake, z (L) is the vertical coordinate, t (T) is time, K (L T^{-1}) is the soil hydraulic conductivity, c (M L^{-3}) is the solute concentration, v_z (L T^{-1}) is the water flux, f (M L^{-3}T^{-1}) is the function for the zero- and first-order rate reactions for solute in the liquid and soil phases, S_c (M L^{-3}T^{-1}) is the root solute uptake, D_z (L^2 T^{-1}) is the dispersion coefficient.

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

$$\Theta = (\theta - \theta_r)/(\theta_s - \theta_r) = [1 + |\alpha h|^n]^{-m} \tag{3}$$

$$K(\theta) = K_s \Theta^{0.5}[1 - (1 - \Theta^{1/m})^m]^2 \tag{4}$$

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

The dispersion coefficient in Eq. (2) is given by Bear (1972)

$$\theta D_z = D_L v_z + \theta D_d \tau \tag{5}$$

where D_d (L^2 T^{-1}) is the ionic molecular diffusion coefficient in free water, D_L (L) is the dispersivity, and τ is the tortuosity factor, which is defined by Millington and Quirk (1961), i.e.

$$\tau = \theta^{7/3} / \theta_s^2 \tag{6}$$

2.2 Explicit algorithm for the governing equations

Eqs. (1) and (2) are partial differential equations which normally requires complex numerical schemes such as the FE method to solve them (Šimůnek et al., 1992). This involves an iterative procedure to obtain the solution to the water flow equation (Eq. 1) by solving the system of linear algebraic equations and a solution to the transport equation (Eq. 2). Yang et al. (2009) have demonstrated that a procedure using an integration strategy of Eq. (1) over the soil layers could result in a much simpler algorithm and satisfactory results in simulating soil water movement. The approach works with soil layers with uniform thickness. The thickness of soil layer is fixed as 5 cm which is considered appropriate and commonly used in agro-hydrological models (Greenwood, 2001; Zhang et al., 2007, 2009; Renaud et al., 2008; Pedersen et al., 2010) to describe processes such as root length distribution in the soil-crop system. In this study, this technique has further been expanded to Eq. (2) so that the simulations of soil water movement and solute transport were made easier. The proposed approach considers that water movement and solute transport in a soil layer is only influenced by the adjacent layers in a small time step, allowing soil water flow and solute transport to be calculated on a layer basis.

Integrating Eq. (1) vertically over a soil layer leads to (Yang et al., 2009)

$$\Delta\theta_i / \Delta t = (v_{w\,i+1} - v_{w\,i}) / \Delta z - S_w \qquad (7)$$

Similarly, using the same scheme to Eq. (2) yields

$$\Delta(\theta_i c_i) / \Delta t = (v_{c\,i+1} - v_{c\,i}) / \Delta z - f - S_c \qquad (8)$$

where i is the soil layer number, Δt is the time step, $\Delta\theta_i$ is the layer-average soil water content change in layer i in Δt, Δz is the soil layer thickness, $v_{w\,i+1}$ and $v_{c\,i+1}$, $v_{w\,i}$ and v_{ci} represent water flux and solute transport from the layer i+1 to i and from i to i-1, which are calculated

$$v_{wi+1} = K_{i+1}(\theta_{i+1})(\Delta h_{i+1,i} / \Delta z + 1) \tag{9}$$

$$v_{ci+1} = (D_L v_{zi+1} + \theta_{i+1} D_d \tau)(\Delta c_{i+1,i} / \Delta z - v_{zi+1} c_{i+1}) \tag{10}$$

$$v_{wi} = K_i(\theta_i)(\Delta h_{i,i-1} / \Delta z + 1) \tag{11}$$

$$v_{ci} = (D_L v_{zi} + \theta_i D_d \tau)(\Delta c_{i,i-1} / \Delta z - v_{zi} c_i) \tag{12}$$

where $\Delta h_{i+1,i}$, $\Delta h_{i,i-1}$ and $\Delta c_{i+1,i}$, $\Delta c_{i,i-1}$ are the differences in soil pressure head and solute concentration between layers *i*+1 and *i*, and *i* and *i*-1, respectively.

To implement the proposed procedure, the soil domain is discretized into 5 cm layers. The bottom layer is numbered 1, and the soil layer number increases upwards to the top layer. Eqs. (7) and (8) are applied from the layer 1 at the bottom to the top layer for the re-distributions of water content and solute concentration in the soil profile at each time step Δt. Detailed steps of implementing the procedure for the soil water movement, which is similar with that for the present work, can be seen elsewhere (Yang et al., 2009)

2.3 Sink and N transformation terms in the soil-crop system

Eqs. (1) and (2) are general equations describing water movement and solute transport in soil. In this study, in addition to the evaluation of the proposed algorithm in modeling soil water movement and solute transport, we also tested the algorithm for predicting water and N dynamics in a soil-wheat system. To do so the sink terms for water and N uptake and N transformation required to be specified.

2.3.1 Sink term for water uptake S_w

The sink term for root water uptake S_w is dependent on crop water demand, root length distribution and soil water availability. It is formulated as (Feddes et al., 1978)

$$S_w = \alpha_w(h)\ L(z)T_{pot} / \Sigma L(z) \tag{13}$$

in which

$$\alpha_w(h) = \begin{cases} 0 & h \le h_3\ , h \ge h_1 \\ (h - h_3)/(h_2 - h_3) & h_3 < h < h_2 \\ 1 & h_2 \le h < h_1 \end{cases} \tag{14}$$

where α_w is the root water stress reduction factor, similar with that by Feddes et al. (1978), T_{pot} (L T^{-1}) is the potential crop transpiration, and L (L L^{-3}) is the root length density. 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, 2010a).

The potential crop transpiration is calculated according to the FAO 56 crop coefficient method (Allen et al., 1998)

$$T_{pot} = K_{cb} ET_0 \tag{15}$$

where K_{cb}, dependent on crop species and its development stage, is the basal crop coefficient for transpiration, ET_0 (L T^{-1}) is the reference evapotranspiration. ET_0 and K_{cb} can be determined according to Allen et al. (1998).

Root growth simulation is in accordance with that proposed by Pedersen et al. (2010). The rooting depth is calculated as a product of the cumulative mean day temperature and the specific root growth rate, while crop total root length is calculated as a product of root dry weight and a fixed specific root length. The root length declines logarithmically from the soil surface downwards (Pedersen et al., 2010), i.e.

$$\Delta L_0 = \Delta W_r S_r \tag{16}$$

$$\Delta R_z = \max[0, \Delta(T - T_{rbase}) K_{rz}] \tag{17}$$

$$L(z) = \begin{cases} L_0 e^{-a_z z} & z < R_z \\ L_0 e^{-a_z z}[1 - (z - R_z)/(0.3R_z)] & R_z \le z \le 1.3R_z \end{cases} \tag{18}$$

where ΔW_r (M L^{-2}) is the increment in root dry weight, which is a function of the increment in crop dry weight and crop dry weight (Zhang et al., 2009), S_r (L M^{-1}) is a specific root length density, ΔR_z and R_z (L) are the increment in rooting depth and the rooting depth, respectively, T (K) is the mean daily air temperature, T_{rbase} (K) is the base temperature for root growth, K_{rz} (L T^{-1} K^{-1}) is the vertical root growth rate, ΔL_0

and L_0 (L) are the increment of root length and the total root length, respectively, and a_z is the shape parameter controlling root distribution down the profile.

2.3.2 Sink term for N uptake S_c

The sink term for N uptake, based on the crop N demand, root length distribution, soil mineral N concentration and the minimum soil mineral N concentration for root uptake, is formulated as (Pedersen et al., 2010)

$$S_c = (U_N + U_{Nr})[1 - e^{-N_{pot}/(U_N + U_{Nr})}] \qquad (19)$$

in which the potential N uptake N_{pot} is estimated by modifying the equation from Nielsen and Barber (1978)

$$N_{pot} = \Sigma L(z) k_N (c_N - c_{N\min})/(c_N + c_0) \qquad (20)$$

where U_N and U_{Nr} (M L^{-2}) are the N demand in the above-ground and root biomass, respectively, N_{pot} (M L^{-2}) is the potential N uptake, c_N (M L^{-3}) is the layer-specific soil mineral N concentration in the 5 cm soil layers, c_{Nmin} (M L^{-3}) is the minimum soil mineral N concentration below which no N uptake is possible, c_0 (M L^{-3}) is the plant N uptake coefficient, and k_N (M L^{-1} T^{-1}) is the plant N uptake efficiency.

2.3.3 N transformation term f

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 first-order. The equation for estimating N released from soil organic matter is given in Zhang et al. (2009) and Zhang et al. (2010b).

$$f = N_{s\min} = k_{\min} Q_{10}^{(T-T_s)/10} \rho Z_{s\min} m_c / R_{CN} \tag{21}$$

where N_{smin} (M L^{-2} T^{-1}) is the daily N mineralization rate from soil organic matter, k_{min} (T^{-1}) is the rate of temperature-independent organic matter breakdown, ρ (M L^{-3}) is the soil bulk density, Z_{smin} (L) 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 (K) is the base temperature at which $Q_{10}^{(T-T_s)/10}$ equals 1, and Q_{10} is the factor change in rate with a 10 degree change in temperature.

2.4 Water flux on the soil surface

The soil surface is subject to the atmospheric condition, i.e. rainfall and potential soil evaporation (irrigation is treated in the same way as rainfall). The potential soil evaporation is estimated using the FAO approach (Allen et al., 1998)

$$E_{pot} = K_e ET_0 \tag{22}$$

where E_{pot} (L T^{-1}) is the potential soil evaporation, and K_e is the evaporation coefficient, which can be calculated using the FAO approach according to the crop species and its development stage (Allen et al., 1998).

In the case of the sum of rainfall and irrigation greater than the potential evaporation, the water flux from the surface is considered as infiltration. The actual infiltration flux in a given time step, ΔI_{act} (L T^{-1}), is determined by the following equation (Yang et al., 2009).

$$\Delta I_{act} = \min[(\theta_s - \theta_{Top})\Delta z / \Delta t, w_{Top}] \tag{23}$$

in which, θ_{Top} is the water content in the top soil layer, and w_{Top} (L T^{-1}) is the potential net water flux at the surface.

Otherwise, the water flux on the soil surface is treated as evaporation, and the actual evaporation in a given time step from the top soil layer, ΔE_{act} (L T^{-1}), is expressed as (Yang et al., 2009)

$$\Delta E_{act} = \min\{K_{Top} \, |(h_{\min} - h_{Top}) / \Delta z + 1|, w_{Top}\} \tag{24}$$

where K_{Top} and h_{Top} are the soil hydraulic conductivity and soil pressure head in the top layer, respectively, and h_{min} (= -26500 cm) is the minimum soil pressure head that the atmosphere could possibly exert in the top soil layer (Yang et al., 2009).

In order to calculate plant transpiration and soil evaporation, daily potential transpiration by plant (Eq. 15) and evaporation from soil surface (Eq. 22) are first calculated. The amounts of transpiration and evaporation in Δt are then determined by evenly distributing daily transpiration and evaporation over 24 h. The calculated potential soil evaporation in Δt is applied to the soil surface for computing actual evaporation, whereas the potential crop transpiration is applied in the root zone for computing actual root water uptake.

It should be pointed out that soil evaporation and plant transpiration are coupled processes, and therefore they should be dealt with simultaneously as implemented in numerical methods such as the FE method. However, in cascade models these processes are decoupled at daily intervals. This leads to a much simpler calculation procedure, but could compromise the estimation of plant transpiration. For example, under the circumstances of soils containing limited water, if soil evaporation is satisfied first, then plant transpiration could be underestimated. In this study, the identical approach for calculating soil evaporation and plant transpiration used in cascade models is adopted, and both transpiration and evaporation are computed in each time step Δt. Since plant transpiration and soil evaporation in each time step are very small (as a result of the small time step of 0.001 d), the error in calculating plant transpiration is greatly reduced. Thus the proposed algorithm has the simplicity and robustness of cascade approaches and accuracy of numerical methods. Moreover, the proposed algorithm, compared with cascade models, has the advantage of considering water infiltration more accurately in the cases where rainfall or irrigation intensity is known in detail (Yang et al., 2009).

2.5 Model evaluation

Model performance is often evaluated using the correlation coefficient (R) or the coefficient of determination (R^2). However, Willmott and Wicks (1980) found that high values of R or R^2 may not be related to the sizes and the differences between measurement and simulation, and thus could in fact be misleading. In this study a more exhaustive approach for an evaluation of model performance was carried out as suggested by Willmott (1982). The calculated metrics on which the model performance was assessed included: the Nash-Sutcliffe efficiency (*NSE*) (Nash and Sutcliffe, 1970), the root of the mean squared error (*RMSE*), and the mean absolute error (*MAE*)

$$NSE = 1 - \sum_{i=1}^{N_o} (P_i - O_i)^2 / \sum_{i=1}^{N_o} (P_i - O^{'})^2 \tag{25}$$

$$RMSE = [N_o^{-1} \sum_{i=1}^{N_o} (P_i - O_i)^2]^{0.5} \tag{26}$$

$$MAE = N_o^{-1} \sum_{i=1}^{N_o} | P_i - O_i | \tag{27}$$

where P_i and O_i are the predicted and measured values, respectively, $O^{'}$ is the average of the measured values, and N_o is the number of measurements.

3. Experiments

The experiment used for testing the fitness of the proposed algorithm was conducted in the Bouwing farm on winter wheat at the Institute for Soil Fertility Research, The Netherlands in 1983 (Groot and Verberne, 1991). The summary of the experiment relevant to this study including fertilization is given in Table 1. The measurements included spatial-temporal soil water content, soil mineral N in the layers of 0-30, 30-60 and 60-90 cm as well as above-ground dry matter accumulation, and N contents in various organs during growth made at intervals of three weeks from February 1983. N contained in the above-ground dry weight was measured at the same time as these for soil water content and mineral N concentration. The weather variables including air temperature, radiation and rainfall were measured during the experiment. Details of the experiment can be seen in Groot and Verberne (1991).

4. Model parameterization

This study was carried out in two parts. The first part examined the proposed algorithm in the simulation of water movement and solute transport in different soils via numerical experiments, and included a comparison of its performance against the FE method. The second part involved comparing of the simulation results using the proposed algorithm for water and N dynamics in the soil-wheat system with the data from the field experiment described above.

4.1 Numerical study

To examine the performance of the proposed algorithm in hydrological simulations, a case of modeling water movement and nitrate transport in a soil column immediately after an application of 100 kg ha^{-1} nitrate-N (NO_3-N) was assumed. The FE method was selected for comparison. The simulations were carried out on three soils: i.e. a coarse, a medium and a fine texture. The hydraulic properties 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 100 cm, with an initial soil water content set to be 0.393, 0.432 and 0.513 cm^3 cm^{-3} throughout the column for the coarse, medium and fine soils, respectively. The lower boundary condition was specified as free drainage, whereas no water flux was allowed at the surface. It was assumed that NO_3-N was dissolved in the top 5 cm soil layer immediately after the application. The calculated NO_3-N concentrations were 0.513, 0.463 and 0.390 mg cm^{-3} for the coarse, medium and fine soils, respectively. The diffusion coefficient and dispersivity were 1.64 cm^2 d^{-1} and 0.5 cm, respectively. For the proposed algorithm, the soil column was divided into 20 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 method, the soil column was divided into 50 soil layers with various thicknesses (thin layers at the bottom where the lower boundary condition was imposed). Two FE methods with and without the 'upstream weighting and the artificial dispersion' scheme, named as the 'complex' and 'ordinary' FE methods, were used in the simulations for comparison.

4.2 Validation experiment

Soil water retention curves for different layers (0-40 and 40-100 cm) in the validation experiment were given in Groot and Verberne (1991). The values of the hydraulic parameters used in Eqs (3) and (4) to describe the soil water retention curves were fitted using the RETC software (van Genuchten et al., 1991) and are listed in Table 3 (after Yang et al., 2009), based on the data provided by Groot and Verberne (1991). The calculated soil domain was 120 cm down from the soil surface, and the boundary condition at the bottom was set as free drainage (Yang et al., 2009).

The soil hydraulic properties in the layer of 100-120 cm were assumed the same as those in the layer of 40-100 cm.

The daily above-ground N requirement was calculated using the following equations which were obtained by differentiating the cumulative N curves fitted based on the measurements given by Groot and Verberne (1991) with respect to time (Fig. 1a)

$$U_N = \begin{cases} 0.077 & 38 \le DOY < 87 \\ 0.0358DOY - 2.6119 & 87 \le DOY < 164 \\ 1.245 & 164 \le DOY \le 213 \end{cases} \qquad \mathrm{kg\,ha^{-1}} \qquad (28)$$

where DOY is the Julian day of the year.

The amount of N partitioned in the roots was estimated using the approach described in Zhang et al. (2009). The increment in root dry weight is a fraction of the increment in the above-ground crop dry weight with the fraction decreasing with an increase in above-ground dry weight. The above-ground dry weight was modeled using a simple growth equation which mimics initial exponential followed by near constant growth. The equation, which is temperature-driven and uses the targeted yield, calculates the daily above-ground dry weight ΔW (t ha^{-1}) as $W/(1+W)$ (Greenwood et al., 1985; Greenwood, 2001). The root %N changes with W in the way of $\%N_{crit} = 1 + 1.35e^{-0.26W}$ (Greenwood et al., 1985; Greenwood, 2001). By setting the measured dry yield of 17 t ha^{-1} as the target yield in the growth equation, the modeled root dry weight and corresponding N amount in the experiment are shown in Fig. 1(b). The modeled ratio of above-ground dry weight to root dry weight at harvest was 0.16, close to the experimental finding of 0.19 (Arima et al., 1999). This, together with the root %N equation which is based on experimental evidence (Osaki et al., 1997), makes the estimation of N partitioned into the roots reliable. Since the variations of N in the roots do not change markedly in the very early stages and towards maturity, only N uptake in roots at the middle growth stages was considered and the uptake rate was 0.42 kg N ha^{-1} d^{-1}. Other parameter values used in the simulations for the validation experiment are shown in Table 4, based on the work by Pedersen et al. (2009) and Zhang et al. (2007; 2009). The weather information used in the simulation periods, including daily mean, minimum and maximum air temperatures, wind speed, rainfall and global radiation, was given in Groot and Verberne (1991).

The simulation started on the first measurements on 7 February 1983 of soil water content and mineral N concentration in the profile. The measured soil water content and mineral N concentration distributions down the profile were set as the initial conditions. The time step for solving the governing equations using the proposed algorithm was 0.001 d, which is the same as suggested by Yang et al. (2009) for 5 cm soil layers.

5. Results and discussion

5.1 Numerical study

5.1.1 Fine and medium soils

Soil water content and NO_3-N concentration distributions at various time intervals were simulated and compared using the proposed algorithm and the FE methods for the fine and medium soils (Figs. 2, 3). It is clear that the profiles predicted by the proposed algorithm agree well with those from the FE methods. It was also found that the simulated results from both the ‘ordinary’ and ‘complex’ FE methods were virtually identical for the fine soil, whereas there were slight differences in the simulated soil NO_3-N concentration between the ‘ordinary’ and ‘complex’ FE methods in the medium soil. This indicates that the ‘ordinary’ FE method may sufficiently be accurate in simulating water movement and solute transport in both soils, and the simple algorithm proposed in this study can achieve the same accuracy of the simulated results as those from the FE methods.

5.1.2 Coarse soil

The same simulations and comparisons were also carried out for the coarse soil (Fig. 4). Further, the statistical metrics including *RMSE*, *NSE*, *MAE* and R^2 were calculated for NO_3-N concentration, and the results are shown in Table 5. The simulated soil water content profiles at intervals using the proposed algorithm are in good agreement with those from the FE methods (Fig. 4a), which confirms that the proposed algorithm is capable of simulating soil water movement in different soils accurately. While the simulated NO_3-N concentration profiles at intervals using the proposed algorithm agree fairly well with those from the ‘complex’ FE method (Fig. 4bcd, Table 5), large discrepancies were observed in the simulated results between the ‘ordinary’ FE method and the ‘complex’ FE method, and between the ‘ordinary’ FE method and the proposed algorithm. The ‘ordinary’ FE method severely underestimated NO_3-N transport in the soil profile, resulting in much higher NO_3-N concentration in the top 20 cm soil layer. This can be attributed to the steep NO_3-N concentration front and the dominant convection in the simulated coarse soil. However, the case studied is a real scenario of the fertilization in a wet soil. This suggests that caution should be taken when using the 'ordinary' FE method in predicting NO_3-N movement, especially in estimating NO_3-N leaching in the coarse soil. The differences in NO_3-N concentration profiles simulated by the proposed algorithm and the 'complex' FE method might be due to the artificial dispersion in the FE method resulting from the 'upstream weighting and the artificial dispersion' scheme.

5.1.3 Effect of dispersion term in NO_3-N transport

Fig. 5 shows NO_3-N concentration distributions down the soil profile after 30 day free drainage simulated using the proposed algorithm for the transport equation with and without the dispersion term. The dispersion term has a bigger effect on NO_3-N transport in the fine and medium soils (Fig. 5bc) than the coarse soil (Fig. 5a). This can be explained by the fact that in the coarse soil NO_3-N transport is dominated by the convection term, i.e. NO_3-N mainly moves with water flow. However, in the medium and fine soils water flow is not as easy as that in the coarse soil due to narrow pores. As a result dispersion becomes an important process in NO_3-N transport in the soil. This implies that in modeling NO_3-N transport in the medium and fine soils, the dispersion term has to be taken into consideration to enable the predictions to be reasonable.

It is evident, from the above, that the proposed algorithm presented in this study produces the results as accurately as those from the ‘complex’ FE method in modeling soil water dynamics and NO_3-N transport in different soils. Given the simplicity, stability and the ability of the proposed algorithm, it can be concluded that the proposed algorithm has a good potential to be used in agro-hydrological models for accurately simulating soil water movement and solute transport.

5.2 Validation experiment

5.2.1 Comparison of simulated and measured soil water content and mineral N concentration

Fig. 6 shows the overall comparisons of the simulated and measured values of soil water content and soil mineral N concentration in the various soil layers at time intervals, whereas Figs. 7 and 8 show the detailed comparisons of the time-course soil water content and mineral N concentration in various layers. The statistical comparisons between the measured and simulated values of soil water content and soil mineral N are given in Table 6. The calculated *RMSE* and *MAE* values for soil water content are 0.038 cm^3 cm^{-3} and 0.032 cm^3 cm^{-3}. Likewise, the values for soil mineral N are 8.95 kg-N ha^{-1} and 5.49 kg-N ha^{-1}. This, and relatively high values of *NSE* of 0.620 and 0.841 for soil water content and soil mineral N, indicates that the overall performance of the model for water and N dynamics in the soil-wheat system was satisfactory. However, a noticeable discrepancy was observed from soil mineral N in the top 30 cm layer on DOY of 164, 31 days after the fertilizer-N application (Fig. 8). The model simulated a sharp increase in soil mineral N in the top 30 cm layer after the fertilization event. But this was not materialized in the measurement. Such a phenomenon of 'disappearance' of the applied fertilizer-N was observed elsewhere (Neeteson et al., 1986; Nielsen and Jensen, 1986), and might be attributed to the soil processes such as ammonia volatilization, denitrification and microbial immobilization which were not considered in this study. Accurate simulations of N transformation in these processes currently remain challenging due to the difficulties in quantifying various factors controlling these processes (Barton et al., 1999; Cannavo et al., 2008).

5.2.2 Simulated water and N dynamics in the soil-wheat system

Actual soil evaporation, crop transpiration and water percolation at 1 m depth were simulated (Fig. 9a). The simulated cumulative soil evaporation and crop transpiration were 108 and 285 mm, respectively. Crop evapotranspiration was mainly met by rainfall during the growing season (344 mm) and soil water originally contained in the soil. Water percolation at 1 m depth was not significant and only occurred at the early crop development stages when the soil was relatively wet (Fig. 9a). The simulated cumulative N uptake, N mineralization from soil organic matter and N leaching at 1 m depth are shown in Fig. 9b. N uptake by the crop before DOY of 100 was small, and followed by a steady increase. N mineralized from soil organic matter accumulated with time, and the accumulation rate increased with time due to the increase in air temperature. During the growing period, the total N mineralized from soil organic matter was 65 kg ha^{-1}. At the end of the simulation the simulated cumulative N uptake was 219 kg ha^{-1}, which was mainly met by the applied fertilizer-N, mineral N originally contained in the soil and the mineralized N from the soil. N leaching at 1m depth was small as the total simulated value was approximately 12 kg ha^{-1}. This was supported by previous studies that in N leaching in the west Europe is not great between spring and autumn when the soil is cropped (Neeteson and Carton, 2001; Zhang et al., 2009).

6. Conclusions

The simple and explicit algorithm for solving the basic soil flow equation (Yang et al., 2009) has been extended to solve the basic solute transport equation using a 5 cm soil layer and a small time step of 0.001 d. Numerical experiments show that the algorithm is able to produce the results as accurately as those from the FE method in modeling soil water dynamics and solute transport, even in the coarse soil where convection is dominated. Compared with the FE method, the proposed algorithm is much simpler, and easier to implement. Thus, the proposed algorithm provides an alternative to the FE method for accurate simulation of water and solute transport in soil using the basic theory. The reliability of the proposal algorithm was also tested in simulating water and N dynamics in the soil-wheat system. Good agreement of the time-course soil water content and mineral N concentration at different depths in the soil profile between measurement and simulation was achieved, suggesting that the proposed algorithm has a potential to be employed in agro-hydrological models.

7. Acknowledgements

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Figure captions:

Fig. 1. Measured N uptake in the above-ground parts (a) and estimated root dry matter and N accumulations (b) in the validation experiment.

Fig. 2. Comparison of soil water content (a) and NO_3-N concentration down the soil profile at intervals (b) for the fine soil.

Fig. 3. Comparison of soil water content (a) and NO_3-N concentration down the soil profile after 5 days (b), 10 days (c) and 30 days (d) for the medium soil.

Fig. 4. Comparison of soil water content (a) and NO_3-N concentration down the soil profile after 5 days (b), 10 days (c) and 30 days (d) for the coarse soil. Key to symbols: see legend to Fig. 3.

Fig. 5. NO_3-N concentration distributions down the soil profile after 30 days calculated with and without dispersion term for the fine soil (a), medium soil (b) and coarse soil (c).

Fig. 6. Overall comparison of soil water content (a) and soil mineral N (b) in different soil layers and at time intervals between measurement and simulation in the validation experiment.

Fig. 7. Comparison of soil water content θ in the layers of 0-30 cm (a) and 30-60 cm (b) and 60-90 cm (c) in the validation experiment.

Fig. 8. Comparison of soil mineral N between measurement and simulation in the layers of 0-30 cm, 30-60 cm and 60-90 cm in the validation experiment (60 kg-N ha^{-1} of N fertilizer was applied on DOY of 133).

Fig. 9. Simulated cumulative actual crop transpiration, soil evaporation and water percolation at 1 m depth (a) and cumulative N uptake, N mineralization from soil organic matter and N leaching at 1 m depth (b) in the validation experiment.

Table 1
Summary of the validation experiment

Soil type	Silty clay loam
Crop	Wheat
Sowing and harvest dates	21 Oct. 1982, 01 Aug. 1983
Layer thickness of measured soil water content and mineral N concentration (cm)	0-30, 30-60, 60-90
Dates of soil water and mineral N measurements (mmdd)	0207,0228,0328,0418,0509,0531, 0613,0704,0718,0801
N fertilizer (kg N ha^{-1}) rate and date of fertilization (mmdd)	(60) 0513

Table 2
Soil hydraulic parameter values for the coarse and fine soils in the numerical experiments (Wösten et al., 1999)

	θ_s (cm^3 cm^{-3})	θ_r (cm^3 cm^{-3})	α (–)	n (–)	K_s (cm d^{-1})
Coarse soil	0.40	0.03	0.0383	1.3744	60.0
Medium soil	0.44	0.01	0.0314	1.1804	12.1
Fine soil	0.52	0.01	0.0367	1.1012	24.8

Table 3

Fitted soil hydraulic parameter values in the validation experiment using the RETC software[a] (Yang et al., 2009)

	θ_s (cm^3 cm^{-3})	θ_r (cm^3 cm^{-3})	α (–)	n (–)	K_s (cm d^{-1})
0–40 cm	0.51	0.00	0.0266	1.1841	40.0
40–100 cm	0.49	0.00	0.0046	1.1835	2.0

[a] The RETC software was developed by van Genuchten et al. (1991).

Table 4
Model parameter values used in the simulations in the validation experiment

Parameter	Value	Unit	Explanation
a_z	3.0	-	Shape parameter for root distribution
c_0	0.007	kg m^{-3}	Mineral N concentration constant
c_{Nmin}	0.002	kg m^{-3}	Min. mineral N concentration in soil layer
k_{min}	0.00015	d^{-1}	Rate of organic matter breakdown
k_N	0.07	g $m^{-1}d^{-1}$	Plant N uptake coefficient
Q_{10}	3	-	Value of Q_{10}
S_r	300000	m kg^{-1}	Specific root length density
T_{max}	27	°C	Max. temperature for root growth
T_{min}	7	°C	Min. temperature for root growth
T_s	20	°C	Base temperature when Q_{10} function equals 1
z_{min}	30	cm	Soil depth where N mineralization occurs

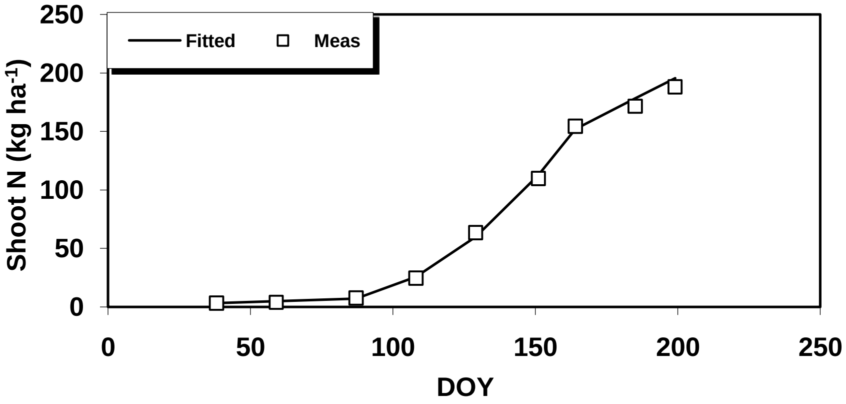
Table 5
Statistical analysis of simulated NO_3-N concentration between the ‘complex’ FE method and the proposed algorithm, and between the ‘complex’ and the ‘ordinary’ FE methods

	RMSE ($mg\ cm^{-3}$)	NSE(–)	MAE ($mg\ cm^{-3}$)	R^2(–)
‘Complex’ FE method vs proposed algorithm	0.022	0.949	0.014	0.965
‘Complex’ FE method vs ‘ordinary’ FE method	0.064	0.585	0.039	0.970

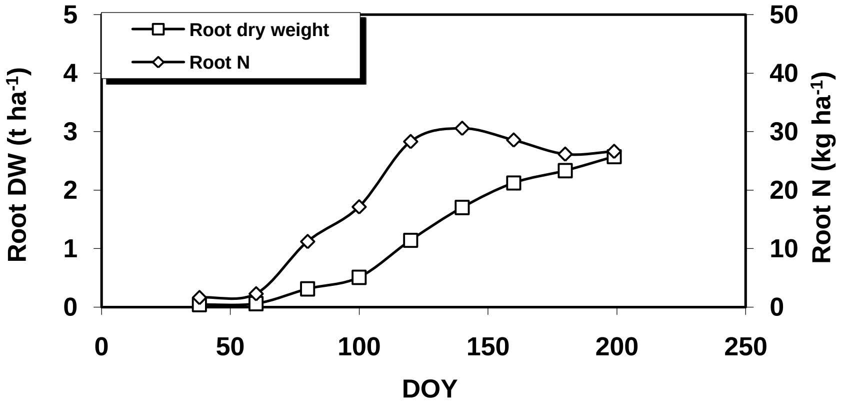
Table 6
Statistical analysis of soil water content and soil mineral N between measurement and simulation

	RMSE[a]	NSE(–)	MAE[a]	R^2(–)
Soil water content (cm^3 cm^{-3})	0.04	0.620	0.03	0.749
Soil mineral N (kg-N ha^{-1})	8.95	0.841	5.49	0.846

[a] RMSE and MAE have the same unit of the analyzed item.


Fitted
Meas
Shoot N (kg ha-1)
250
200
150
100
50
0
0
50
100
150
200
250
DOY

(a)


Root dry weight
Root N
Root DW (t ha-1)
Root N (kg ha-1)
5
4
3
2
1
0
50
40
30
20
10
0
0
50
100
150
200
250
DOY

(b)

Fig. 1

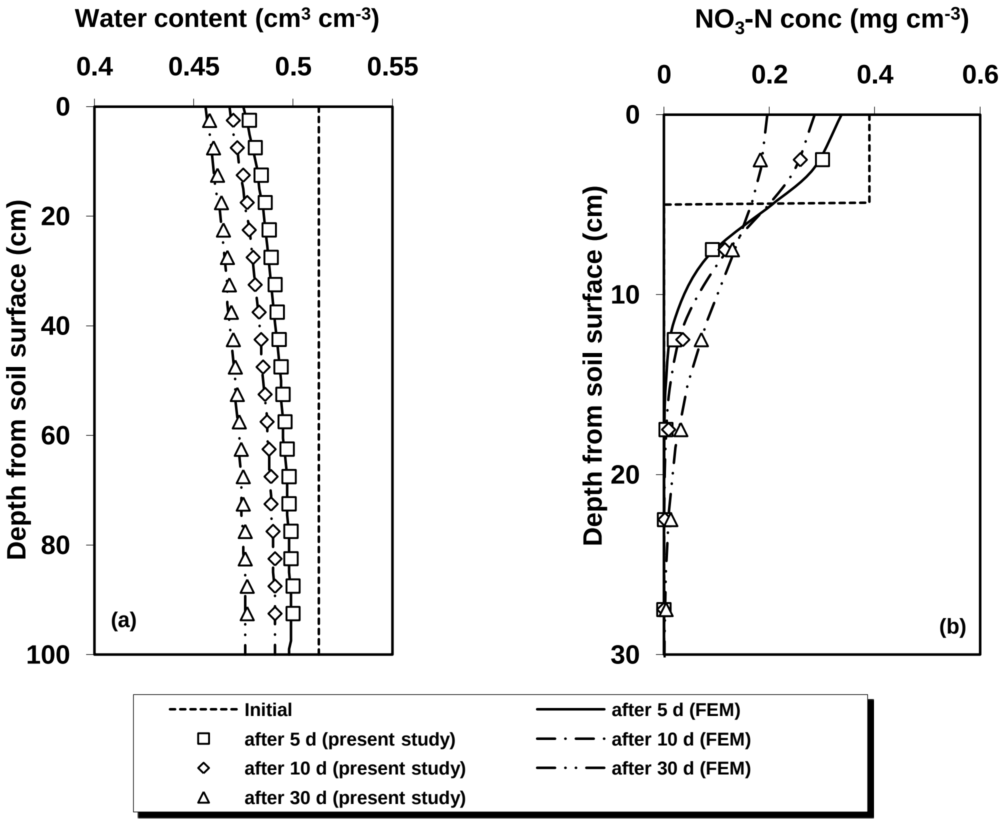

Water content (cm3 cm-3)
0.4
0.45
0.5
0.55
Depth from soil surface (cm)
0
20
40
60
80
100
(a)
NO3-N conc (mg cm-3)
0
0.2
0.4
0.6
Depth from soil surface (cm)
0
10
20
30
(b)
Initial
after 5 d (present study)
after 10 d (present study)
after 30 d (present study)
after 5 d (FEM)
after 10 d (FEM)
after 30 d (FEM)

Fig. 2

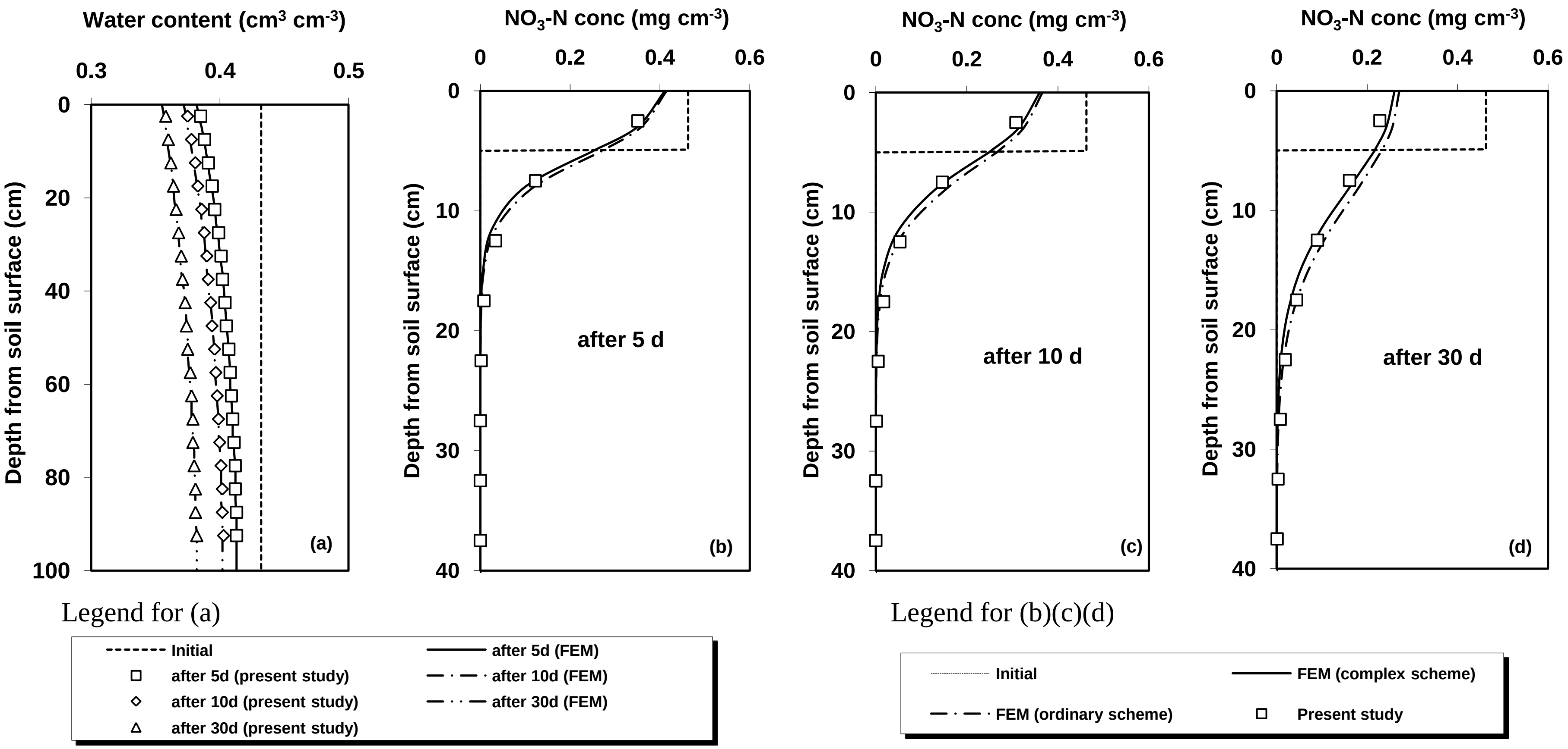

Water content (cm³ cm⁻³)
0.3
0.4
0.5
Depth from soil surface (cm)
0
20
40
60
80
100
(a)
NO₃-N conc (mg cm⁻³)
0
0.2
0.4
0.6
0
10
20
30
40
after 5 d
(b)
after 10 d
(c)
after 30 d
(d)
Legend for (a)
Initial
after 5d (present study)
after 10d (present study)
after 30d (present study)
after 5d (FEM)
after 10d (FEM)
after 30d (FEM)
Legend for (b)(c)(d)
Initial
FEM (complex scheme)
FEM (ordinary scheme)
Present study

Fig. 3

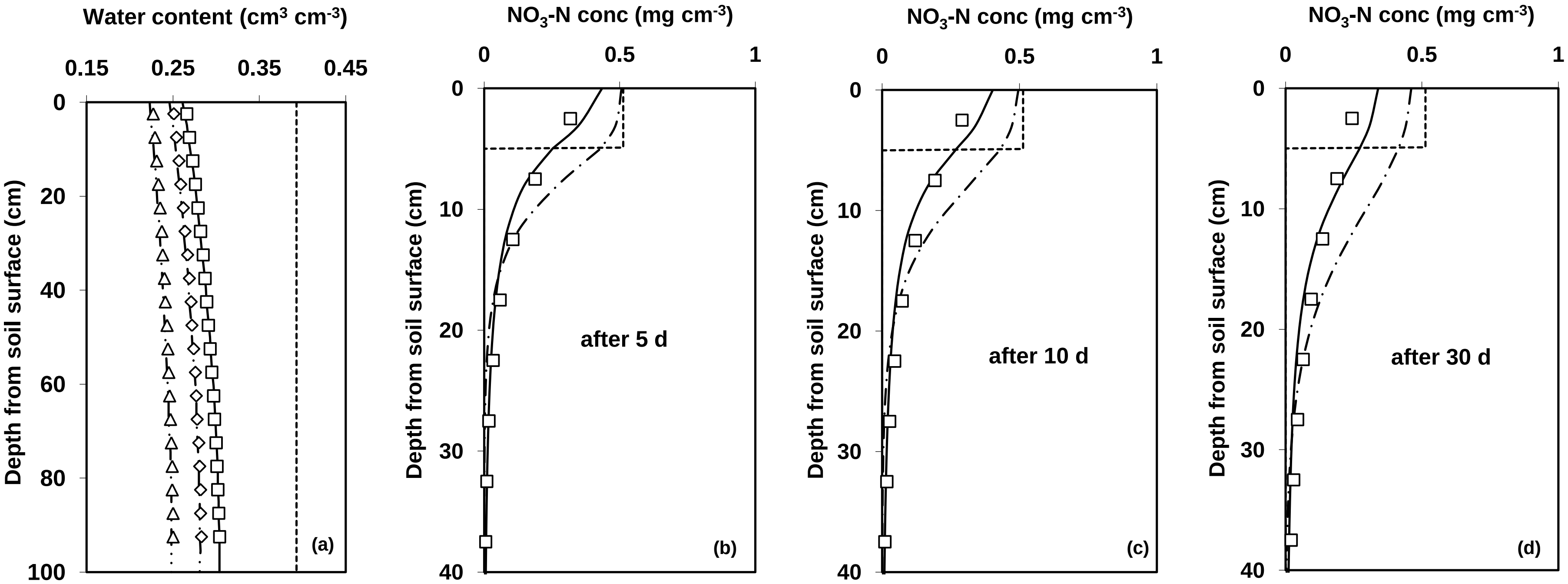

Water content (cm^3 cm^{-3})
0.15
0.25
0.35
0.45
0
20
40
60
80
100
Depth from soil surface (cm)
(a)
NO$_3$-N conc (mg cm^{-3})
0
0.5
1
0
10
20
30
40
after 5 d
(b)
after 10 d
(c)
after 30 d
(d)

Fig. 4

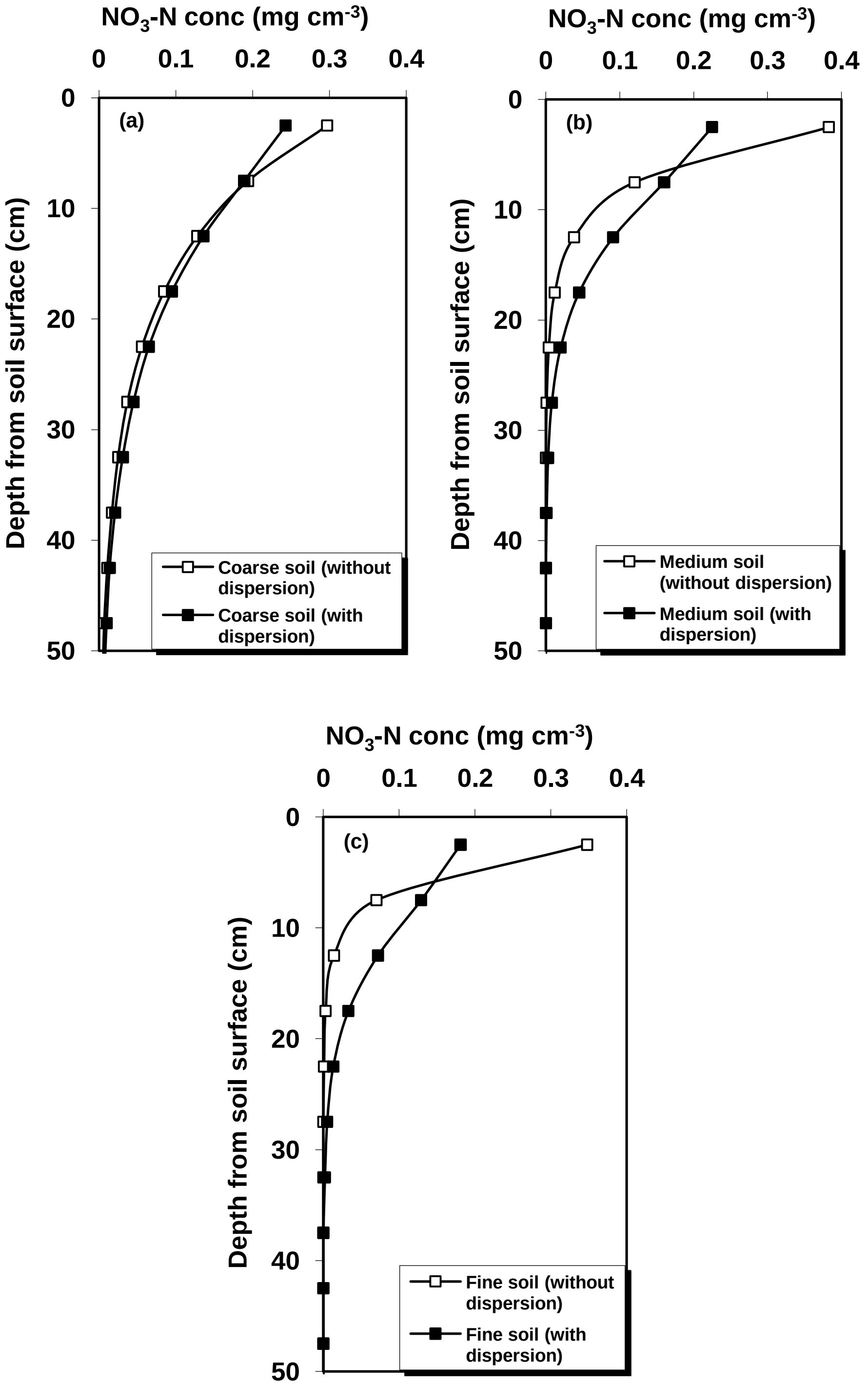
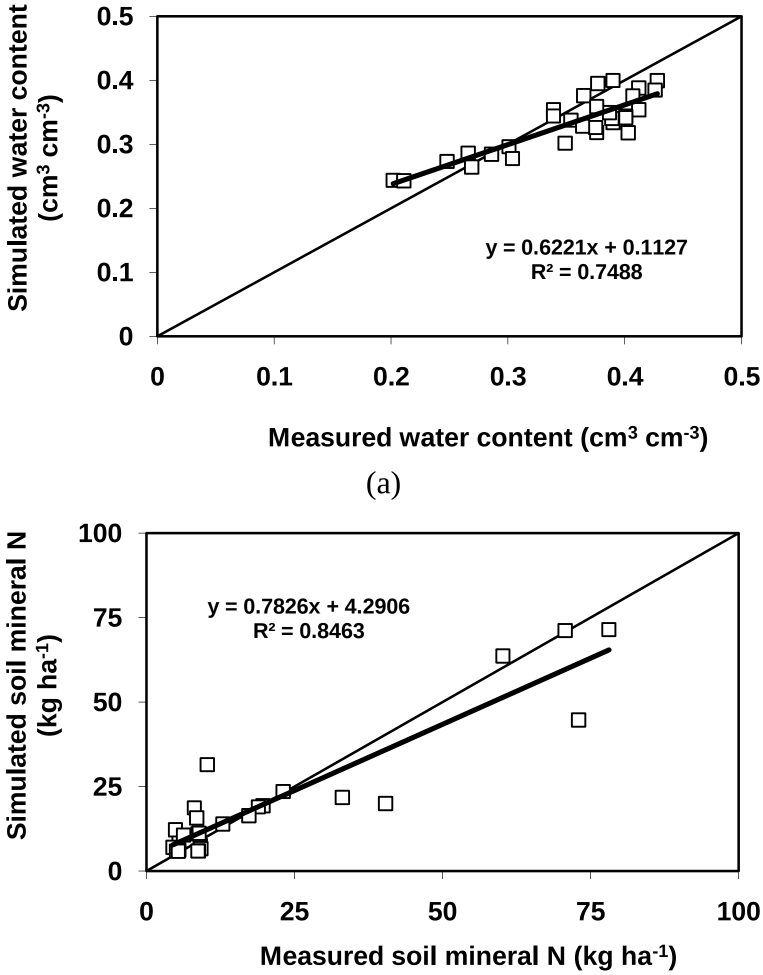

NO3-N conc (mg cm-3)
0
0.1
0.2
0.3
0.4
Depth from soil surface (cm)
0
10
20
30
40
50
(a)
Coarse soil (without dispersion)
Coarse soil (with dispersion)
(b)
Medium soil (without dispersion)
Medium soil (with dispersion)
(c)
Fine soil (without dispersion)
Fine soil (with dispersion)

Fig. 5


Simulated water content (cm^3 cm^{-3})
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
y = 0.6221x + 0.1127
R² = 0.7488
Measured water content (cm^3 cm^{-3})
Simulated soil mineral N (kg ha^{-1})
100
75
50
25
0
0
25
50
75
100
y = 0.7826x + 4.2906
R² = 0.8463
Measured soil mineral N (kg ha^{-1})

(a)

(b)

Fig. 6

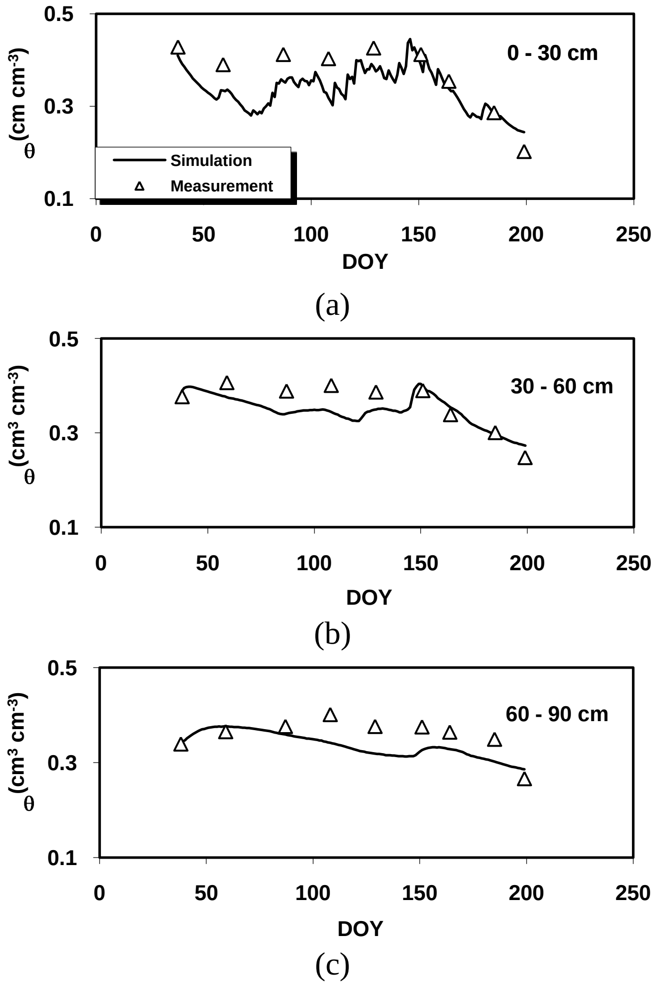
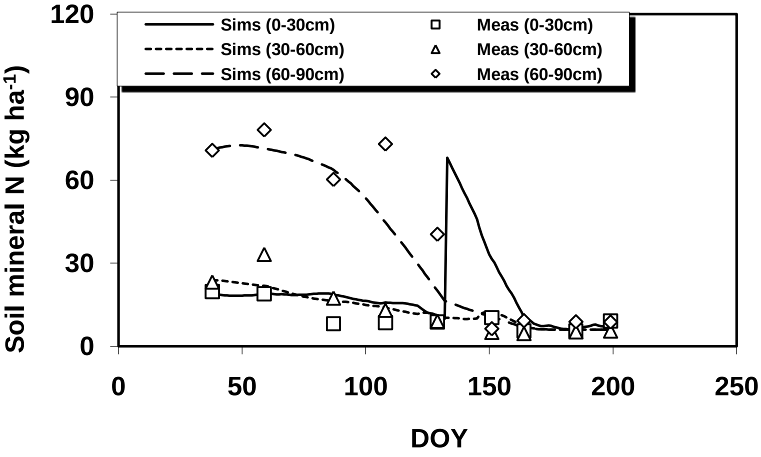
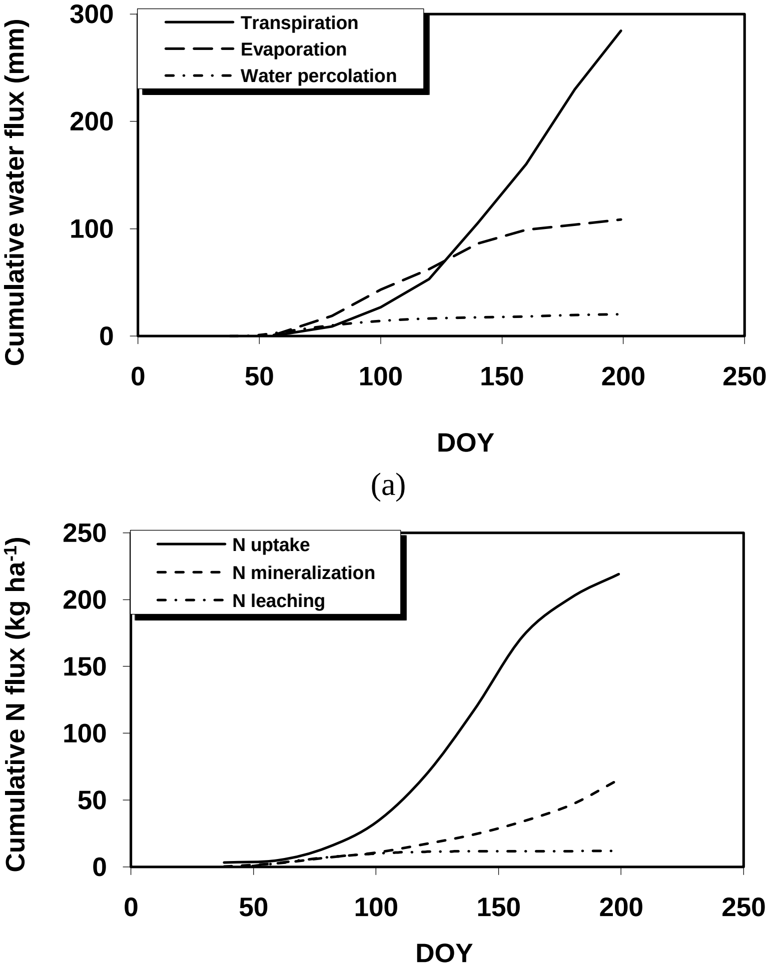

0 - 30 cm
Simulation
Measurement
θ (cm cm^{-3})
0.5
0.3
0.1
0
50
100
150
200
250
DOY
(a)
30 - 60 cm
θ (cm^3 cm^{-3})
(b)
60 - 90 cm
(c)

Fig. 7



Sims (0-30cm)
Sims (30-60cm)
Sims (60-90cm)
Meas (0-30cm)
Meas (30-60cm)
Meas (60-90cm)
Soil mineral N (kg ha-1)
120
90
60
30
0
0
50
100
150
200
250
DOY

Fig. 8


Cumulative water flux (mm)
300
200
100
0
Transpiration
Evaporation
Water percolation
0
50
100
150
200
250
DOY
Cumulative N flux (kg ha-1)
250
200
150
100
50
0
N uptake
N mineralization
N leaching
0
50
100
150
200
250
DOY

(a)

(b)

Fig. 9