



## Transient three-dimensional modeling of soil water and solute transport with simultaneous root growth, root water and nutrient uptake

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### Abstract

A three-dimensional solute transport model was developed and linked to a three-dimensional transient model for soil water flow and root growth. The simulation domain is discretized into a grid of finite elements by which the soil physical properties are spatially distributed. Solute transport modeling includes passive and active nutrient uptake by roots as well as zero- and first-order source/sink terms. Root water uptake modeling accounts for matric and osmotic potential effects on water and passive nutrient uptake. Root age effects on root water and nutrient uptake activity have been included, as well as the influence of nutrient deficiency and ion toxicity on root growth. Examples illustrate simulations with different levels of model complexity, depending on the amount of information available to the user. At the simplest level, root growth is simulated as a function of mechanical soil strength only. Application of the intermediate level with root water and nutrient uptake simulates the influence of timing and amount of NO<sub>3</sub> application on leaching. The most comprehensive level includes simulation of root and shoot growth as influenced by soil water and nutrient status, temperature, and dynamic allocation of assimilate to root and shoot.

### Introduction

The efficiency in the utilization of below-ground resources by the root system plays an important role in determining crop yield (Andren et al., 1993). Nutrients and other soluble substances move to roots by diffusion and mass flow induced both by soil water and nutrient status and by root water and nutrient uptake. However, the extent and shape of the root system and their changes with time also play a major role in determining uptake patterns. Therefore, along with the characteristics of the soil nutrient supply, it is important to understand root growth dynamics and activity (van Noordwijk and de Willigen, 1991).

Nutrient uptake efficiency can be important also in explaining changes in the chemistry of both soils and drainage waters. Processes like soil salinization and

ion accumulation in the soil to toxic levels are affected by plant evapotranspiration and root uptake. Through the process of root uptake, plants can remove saline and/or toxic ions from the soil. For example, Ben-Asher (1994) modeled Se uptake by selected plant species, determining the maximum Se concentration allowed for Se-resistant plant growth and evaluating the efficiency of Se removal through uptake.

Surveys on fertilization practices during the past 40 years have demonstrated a steady yearly increase in the total amounts of fertilizers used. For example, the rate of N application to corn fields in the United States has increased 5 times more than the corresponding N content in harvested corn grains, indicating that N is lost mainly through other pathways such as microbial and chemical activities and leaching. A fine-tuning of fertilizer application is crucial for both economical and environmental reasons. Near-maximum crop

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production can be achieved while simultaneously reducing farming costs and decreasing leaching of agricultural chemicals from the root zone (Shaviv and Mikkelsen, 1993).

Thus, an improved understanding of shoot-root-soil relationships has become essential in modern agriculture. Uptake of chemicals by the root system depends mainly on two factors. These are the characteristics of the root system (e.g. morphology, growth rate, nutrient absorption rate) and the interaction of the chemical species with the soil and the soil-water supply (e.g. soil adsorption, mass transport, diffusion). In recent years, several mathematical models have been developed to simulate root growth and its interaction with both the soil water and nutrient supply. However, most of these models have used simplified forms of the equations describing soil water flow and solute transport, and have failed to address issues which may play a key role in a more realistic description of shoot-root-soil continuum, such as effects of root age and decay on water and solute uptake, solute-uptake mechanisms, soil physical variability, transient soil water flow, and soil-solution chemistry.

Modeling root nutrient uptake started with simulation of mass flow and diffusion of nutrients to a single root, approximated by a cylinder of constant radius, solving a simple form of the convection-dispersion equation for a circular geometry (Passioura and Frère, 1967) considering water but no nutrient uptake. Nye and Marriott (1969) included nutrient uptake, using a Michaelis-Menten type boundary condition at the soil-root interface, and explored the sensitivity of the solution to changes in some of the equation parameters (i.e. diffusion coefficient, soil buffer capacity, root absorbing power and nutrient flux at the root surface), whereas Barley (1970) simulated uptake in a system of irregular, parallel roots. Later models have included root competition (Baldwin et al., 1973) and root growth (Claassen and Barber, 1976; Barber and Cushman, 1981), but the root system was modeled only in terms of root length per unit depth, and no attention was paid to the interaction between three-dimensional distribution of the roots and water and solute transport patterns. Advances have also been made in the modeling of root growth, including the analytical approach of Hackett and Rose (1972a, b), the numerical simulations of Lungley (1973), the three-dimensional simulation models of Diggle (1988) and Pages et al. (1989), and the stochastic approach of Jourdan et al. (1995).

Coupling of such efforts as presented above has led to models capable of simulating various aspects of root-soil dynamics. Models have been developed focusing on the transport and uptake of highly immobile nutrients transported mainly by diffusion (Silberbush and Barber, 1984; Amijee et al., 1991) or mobile nutrients such as nitrate moving through the soil mainly by mass flow. Jones et al. (1991) simulated one-dimensional root growth of a user-selected crop as influenced by soil physical properties, soil water and nutrient content, and temperature. Clausnitzer and Hopmans (1994) simulated three-dimensional root architecture and the interaction between root growth and soil-water movement, emphasizing the effects of soil strength on root growth, whereas Benjamin et al. (1996) modeled the influence of rooting patterns on root-water uptake and leaching in two dimensions.

The objective of this study was to develop a transient model for the simultaneous dynamic simulation of water and solute transport, root growth, and root water and nutrient uptake in three dimensions. The three-dimensional water flow and root growth model by Clausnitzer and Hopmans (1994) was expanded to simulate solute transport and nutrient uptake, and the interaction between plant growth and nutrient concentration, thus providing a tool for studying the dynamic relationships between changing soil-water and nutrient status and root activity. The model presented offers the most comprehensive approach to date in the modeling of the dynamic relationship between root architecture and soil domain. The convection-diffusion equation used for modeling of nutrient transport was considered in its most complete form, thus allowing a realistic description of solute fate in the soil domain. Root water uptake is computed as a function of matric and osmotic potential, whereas absorption of nutrients by the roots can be calculated as a result of passive and active (Michaelis-Menten) uptake mechanisms. Uptake and respiration activities can vary along the root axis and among roots as a result of root age. Genotype-specific and environment-dependent root growth processes are described using empirical functions, the latter designed to be easily modified, thus allowing the user to test different formulations and/or introduce new relationships. Although this paper describes the essential features of the model, its size and complexity force us to refer to the report by Somma et al. (1997) for a complete description of the model.

## Model description

The finite-element model (FEM) simulates the growth and activity of a root system as a function of local soil water and nutrient conditions. The domain, treated as a continuum for the modeling of root growth, is discretized into a rectangular grid of finite elements, which serves to describe the spatial distribution of soil physical properties and as a framework for the modeling of transient water flow and solute transport. The FEM adjusts simulation time increments based on convergence of the flow and transport model solution and on root growth time intervals.

Root growth is simulated starting from a germinated seed or using a root system already developed in an earlier simulation. Roots "grow" at user-defined time intervals with a new segment added to the apex of each growing root. The model tracks each segment by recording its topological position within the root system and its spatial location within the model domain, as well as its age, mass and surface area.

At the present stage, the water flow and solute transport model interacts with root growth at one of three different levels of increasing complexity, depending on the simulation objective or how much information is available to the user. These levels are: root growth as a function of soil strength and nutrient concentration, without root water and nutrient uptake (level 1); root growth with potential transpiration defined as a function of time, with or without nutrient uptake (level 2); and root growth with dynamic assimilate allocation to shoot and root, with or

without nutrient uptake (level 3). Table 1 summarizes the options available at each simulation level.

Mass-balance calculations were included for both water flow and solute transport to: (i) evaluate the performance of the numerical solution schemes, and (ii) provide quantitative information on water and nutrient input, root uptake, and water and nutrient leaching. Two different root-water extraction functions have been included in the model, with the possibility of taking into account osmotic potential effects on water and passive nutrient uptake. The model simulates root-age effects on root water and nutrient uptake, as well as the influence of nutrient deficiency or ion toxicity on root growth.

The model source code is almost entirely based on the FORTRAN77 standard, and has been tested for Microsoft FORTRAN Powerstation on a PC. Upon request, the code can be obtained from the authors, together with a user manual describing in detail the structure of the model, the input and output requirements and the pre- and postprocessing software (Somma et al., 1997).

## Mathematical formulation

### Soil water flow

Numerous studies have been published addressing different issues in the modeling water flow in the unsaturated zone using the Richards (1931) equation. A comprehensive review was published Milly (1988), whereas Mariño and Tracy (1988) offered a review of root-water uptake modeling in combination with Richards equation solutions.

The model by Clausnitzer and Hopmans (1994) uses a finite-element, Picard time-iterative numerical scheme (Vogel, 1987; Simůnek et al., 1992) to solve Richards' equation for soil water pressure head  $h$  [L] (negative in unsaturated porous media) in multiple dimensions:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[ K \left( (K_{ij}^A \frac{\partial h}{\partial x_j} + K_{i3}^A) \right) \right] - S \quad (1)$$

where  $\theta$  [L<sup>3</sup>L<sup>-3</sup>] is volumetric soil-water content,  $t$  is time,  $K$  [LT<sup>-1</sup>] is the unsaturated soil hydraulic conductivity,  $K_{ij}^A$  is the generic component of the dimensionless anisotropy tensor for the unsaturated conductivity ( $i, j = 1,2,3$ ),  $x_i$  is the spatial coordinate (L), and  $S$  [L<sup>3</sup>L<sup>-3</sup>T<sup>-1</sup>] is the sink term to account for root water uptake. Choice of boundary conditions

Table 1. Model options for simulation of root growth without solute transport modeling (a) and with solute transport modeling (b).

Features	Simulation levels					
	1a	1b	2a	2b	3a	3b
Water flow	✓	✓	✓	✓	✓	✓
Soil strength	✓	✓	✓	✓	✓	✓
Soil temperature	✓	✓	✓	✓	✓	✓
Ion deficiency/toxicity	✓	✓	✓	✓	✓	✓
Water uptake			✓	✓	✓	✓
Osmotic potential			✓	✓	✓	✓
Root aging and decay			✓	✓	✓	✓
Nutrient uptake				✓		✓
Soil strength effects on plant growth					✓	✓
Concentration effects on plant growth						✓

has been expanded to include a unit hydraulic gradient condition at the bottom boundary, in addition to user-specified, time-varying source/sink volumetric flow rate and pressure head boundary conditions.

### Solute transport

A finite-element model was developed to solve the three-dimensional form of the convection-diffusion equation for solute concentration  $c$  [ML<sup>-3</sup>], derived from Šimunek et al. (1992):

$$\frac{\partial \theta c}{\partial t} + \frac{\rho k \partial c}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho k c + \gamma_w c + \gamma_s \rho - S' c \quad (2)$$

where  $\rho$  [ML<sup>-3</sup>] is the soil bulk density,  $k$  [L<sup>3</sup>M<sup>-1</sup>] is the linear adsorption coefficient,  $D_{ij}$  [L<sup>2</sup>T<sup>-1</sup>] is the generic component of the dispersion coefficient tensor,  $q_i$  [LT<sup>-1</sup>] is the volumetric flux component in the  $i$ -th direction,  $\mu_w$  [T<sup>-1</sup>] and  $\mu_s$  [T<sup>-1</sup>] are the first-order rate constants for the liquid and solid phase respectively,  $\gamma_w$  [ML<sup>-3</sup>T<sup>-1</sup>] and  $\gamma_s$  [T<sup>-1</sup>] are the zero-order rate constants for the liquid and solid phase respectively, and  $S'c$  [ML<sup>-3</sup>T<sup>-1</sup>] is the sink term to account for root solute uptake. The four zero- and first-order rate constants account for reactions of the solute in the dissolved or adsorbed phase, such as microbial degradation, volatilization and precipitation. Simultaneous numerical solutions of Eq. (1) and (2) in its various forms have been presented by Tracy and Mariño (1989) and many others.

For the present model, spatial integration of Eq. (2) was performed using the Galerkin finite-element approach with linear basis functions, while time derivatives were approximated using the finite-difference method. Details about the main steps in the numerical solution of Eq. (2) can be found in Somma et al. (1997). Numerical oscillations of the solution due to the spatial or temporal resolution of the FEM scheme were avoided by reducing the simulation time step based on the product of the Peclet and the Courant numbers as in Perrochet and Berod (1993). To verify the mathematical accuracy of the solute transport model, simple scenarios were simulated in one, two and three dimensions, and solutions were compared to analytical solutions reported by van Genuchten and Alves (1982), Javandel et al. (1984), and Leij and Bradford (1991).

### Water and solute mass balance

To evaluate the accuracy of the numerical solution scheme, water and solute mass balances are computed at each time step, following Šimunek et al. (1992). As part of the mass balance, the absolute cumulative error in the soil water mass balance,  $a^w$  [L<sup>3</sup>], between  $t = t_0$  and  $t = t_1$ , is calculated from:

$$a^w = V_{t_1} - V_{t_0} + \int_{t_0}^{t_1} T_a L_{t_1} dt - \int_{t_0}^{t_1} \sum_{n\Omega} Q_n dt \quad (3)$$

where  $V_{t_1}$ , and  $V_{t_0}$  [L<sup>3</sup>] denote the volumes of water in the simulation domain at times  $t_1$  (current simulation time) and at the beginning of the simulation, respectively. The third term accounts for the cumulative volume of water [L<sup>3</sup>] extracted by the root system,  $T_a$  [L<sup>3</sup>L<sup>-3</sup>T<sup>-1</sup>] being the uptake rate, and  $L_{t_1}$ , [L<sup>3</sup>] the volume of soil occupied by the root system at time  $t_1$ . The fourth term accounts for the cumulative volume of water [L<sup>3</sup>] leaving or entering the flow domain through the boundaries and the internal sources/sinks. Similarly, the absolute cumulative error in the solute mass balance,  $a^c$  [M], is calculated as:

$$a^c = M_{t_1} - M_{t_0} + \int_{t_0}^{t_1} \sum_{n\Omega} Q_n^T dt - M^0 - M^1 - M_r \quad (4)$$

where  $M_{t_1}$  [M] and  $M_{t_0}$  [M] refer to the total mass of solute in the simulation domain at times  $t_1$  and  $t_0$ , respectively, and the third term represents the net cumulative mass of solute [M] moving through the domain boundaries and the internal sources and sinks.  $M^0$  [M] and  $M^1$  [M] denote the mass of solute removed from the domain by zero-order and first-order reactions, respectively, and  $M_r$  [M] corresponds to the mass of solute removed by the root system.

### Root growth

Root growth is simulated as a function of mechanical soil strength, soil temperature and solute concentration. Root axes are generated at user-defined times. Branching time and spacing are described by user-defined functions of root age and branching order (Clausnitzer and Hopmans, 1994).

An impedance factor,  $imp_s$ , is calculated for each growing root apex as a function of the local soil strength conditions at each time  $t$  to reduce the length of the growing segment from its potential (unimpeded)

value. The impedance factor varies linearly between zero (soil strength at which growth ceases completely) and unity (unimpeded growth). An option is available to account for the effects of soil temperature on root growth using the impedance function  $imp_t$ , which varies between zero (temperature at which root growth ceases) and unity (optimal root growth temperature), and is described by a modified sine-wave shape (Clausnitzer and Hopmans, 1994).

Root growth rates are unaffected by nutrient availability as long as the latter is maintained within an optimal concentration range ( $c_{optmin} \leq c \leq c_{optmax}$ ). Because optimal range and minimum and maximum concentration are both genotype- and nutrient-specific, nutrient-concentration effects were simulated using a piecewise linear impedance function,  $imp_c$  [-]. The function varies linearly between zero ( $c \leq c_{min}$  or  $c_{max} \leq c$ , no growth) and unity (optimal concentration range, no impedance). Thus, at each growth event the actual length of the root segment added to each apex is obtained multiplying the unimpeded length with the three current values of the impedance factors  $imp_c$ ,  $imp_s$ , and  $imp_t$ . As nutrient uptake by the roots is not considered at this level of simulation, solute transport is not influenced by the presence of the root system, but is included in the simulation to determine nodal values of the impedance function  $imp_c$ . Alternatively, the nutrient concentration effects on root growth can be evaluated by specifying a time-independent concentration distribution.

Bloom et al. (1993) concluded that root biomass production of field-grown tomatoes is optimal at intermediate levels of soil nitrate and ammonia when all other growth-controlling parameters (water supply, temperature, other nutrient availability) are nonlimiting. Insufficient nutrient supply significantly reduces plant transpiration and photosynthesis (Stark, 1992). Root biomass and growth rate decrease if the nutrients supply is inadequate (de Willigen and van Noordwijk, 1987; Bloom et al., 1993; Shedley et al., 1995). Thus, root growth increases as more nitrogen is available. However, excessive nutrient availability can also hamper plant growth through several mechanisms. For example, Bloom et al. (1993) hypothesized that in the presence of high levels of soil nitrogen root growth becomes carbohydrate-limited. Similar findings were reported by Shedley et al. (1995) for eucalyptus. Wheeler and Power (1995) studied the toxic effects of increasing concentration of trace minerals (Mn, Zn, Cu, B, Fe, Ga, La) in soil solution on wheat.

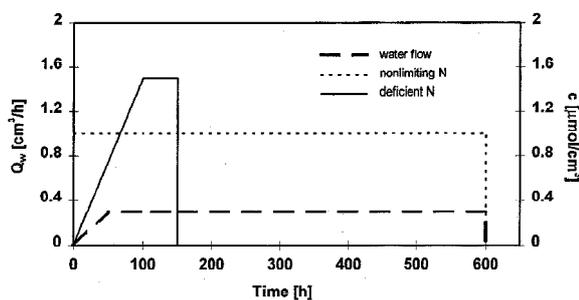


Figure 1. Water and nitrogen application regime for the 'level 1' simulation.

Drew et al. (1975) showed that increasing nutrient supply for only part of the root system of a barley plant increases root growth locally when the rest of the root system is subjected to limited nutrient concentrations. Such effects were simulated with a 'level 1' option to grow barley with two different N application regimes, using the simulation control parameters and soil hydraulic and solute transport parameters presented in Table 2 and Appendix I, respectively. Root growth parameters are presented in Appendix I. Soil temperature was assumed to be optimal.

Both water and  $\text{NO}_3\text{-N}$  were supplied through a dripper, simulated by five nodes at the center of the upper boundary of the simulation domain. For each of those nodes, water flow and solute transport boundary conditions (water flux,  $Q_w$  [ $\text{cm}^3/\text{h}$ ], and concentration,  $c$  [ $\mu\text{mol}/\text{cm}^3$ ], respectively) are presented in Figure 1, whereas initial conditions are presented in Appendix I. A no-flow boundary condition was applied to all the other boundary nodes. Figures 2a and 2b show the simulated root system grown under nonlimiting and deficient  $\text{NO}_3\text{-N}$  supply, respectively. The figure presents conditions at the end of the growth period (25 days). In both cases the soil-water content was such that soil strength did not limit root growth. Root density is presented to the left of each root system, whereas the  $\text{NO}_3\text{-N}$  concentration profile is shown at the right. In the example of Figure 2a,  $\text{NO}_3\text{-N}$  was applied continuously with the irrigation water throughout the growth period. The predicted N-concentration was higher in the upper part of the simulation domain, decreasing downwards. Similarly, the predicted root density decreased with increasing depth. In Figure 2b,  $\text{NO}_3\text{-N}$  was applied only during a limited time interval at the beginning of the growth period (the first 150 hours). Once N application stopped, the subsequent irrigation by the dripper moved the N plume downwards, causing a greater root

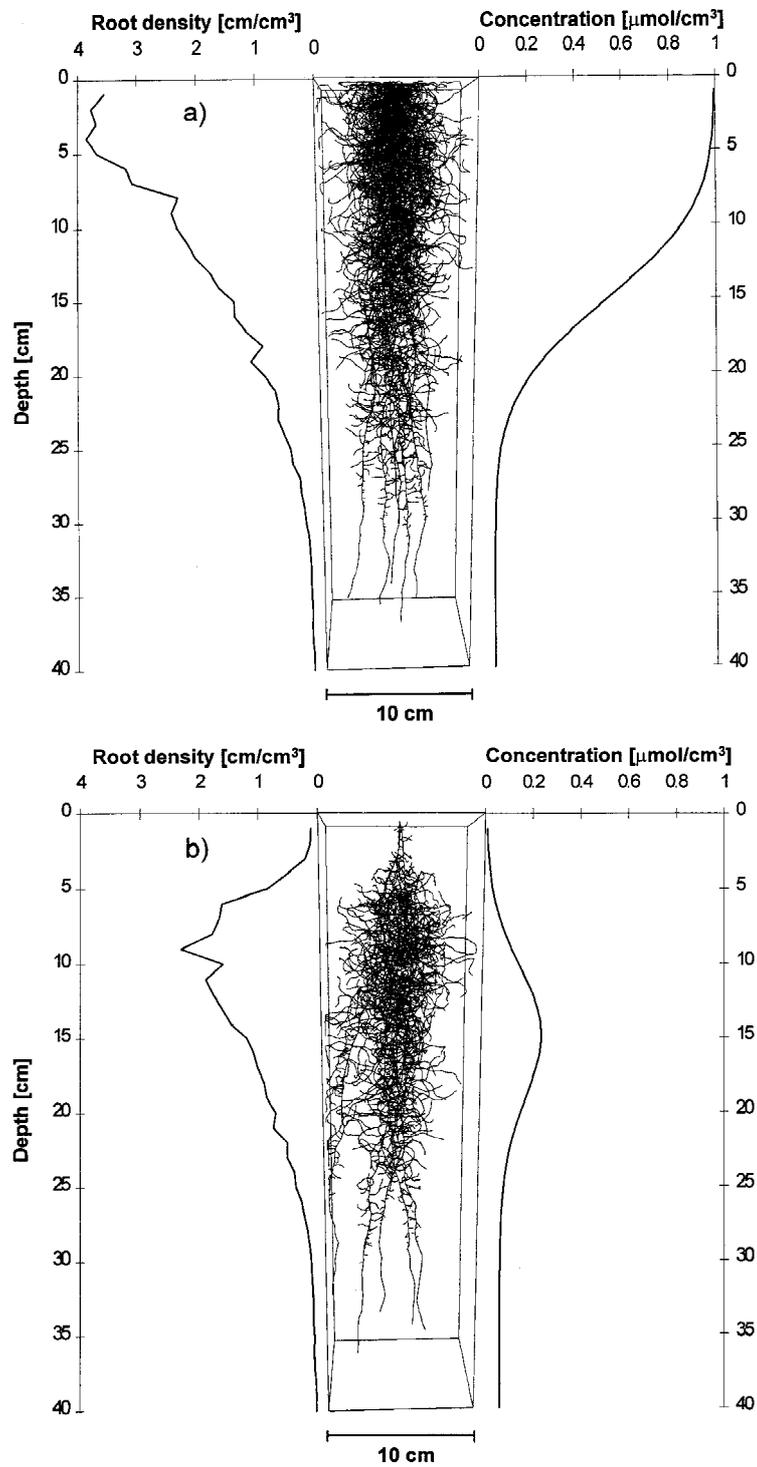


Figure 2. Simulated three-dimensional root architecture with corresponding root density distribution, and nitrogen concentration distribution for 'level 1' simulations: a) non-limiting nitrogen supply and b) deficient nitrogen conditions.

Table 2. Simulation control parameters for simulation levels '1', '2' and '3'

	Figure		
	1,2	3,4,5	6
Simulation level:	1	2	3
Domain size [cm]:	10×10×40	10×10×30	10×10×40
Number of nodes:	11×11×41	11×11×31	11×11×41
Root growth time step [h]:	12	12	12
Simulation end time [h]:	600	600	600

density in the central part of the root zone where the NO<sub>3</sub>-N content was higher. Indeed, the higher predicted root density in the center of the root system was fostered by the higher N amount transported downwards earlier in the simulation, thus explaining the slight offset between root density and N concentration peaks. Thus, the downward movement of the N plume promoted root development at increasing depth, but resulted in a smaller average root density than for the nonlimiting-N case (0.664 cm/cm<sup>3</sup> versus 1.25 cm/cm<sup>3</sup>).

#### Water and solute uptake

The effects of soil salinity on root growth, root water uptake and plant transpiration have been extensively studied. Maas and Hoffman (1977) concluded that crops tolerate salinity up to a threshold level, above which plant yield decreases approximately linearly with increasing salt concentration. Al-Khafaf et al. (1990) studied the response of barley root and shoot growth for various levels of water and/or salinity stress. They concluded that increasing the soil-water osmotic potential reduced evapotranspiration and growth, and causes significant variations in the soil water content distribution. Schmidhalter and Oertli (1991) conducted similar studies on carrots, and concluded that yield decreases linearly with increasing soil salinity for non-limiting water supply conditions. Transpiration rates were affected only at the highest salinity levels, but water stress reduced nutrient uptake due to transport limitations in the soil and restricted root development.

The sink term  $S(x, y, z, t)$  in Eq. (1) is computed from:

$$S(x, y, z, t) = \alpha(x, y, z, t)\beta'(x, y, z, t)T_{pot} \quad (5)$$

where  $\beta'$  is the normalized nodal value of  $\beta$

$$\beta' = \frac{\beta(x, y, z)}{\int_D \beta(x, y, z) dD} \quad (6)$$

and  $D$  denotes integration over the complete soil domain. The set of nodal sink-term values  $S(x, y, z, t)$  was calculated at each time step as in Clausnitzer and Hopmans (1994). However, the localized form of the water-extraction function  $\alpha(x, y, z, t)$  [-], accounting for the local influence of soil-water potential on root water uptake rate, was replaced to include the effects of osmotic potential on root water uptake. The nodal values of  $\alpha(x, y, z, t)$  in the present model were calculated using the expression proposed by van Genuchten (1987), considering the combined effects of matric and osmotic potential on water uptake rate:

$$\alpha(x, y, z, t) = \frac{1}{[1 + (h/h_{50})^{p_1}] * [1 + (\pi/\pi_{50})^{p_2}]} \quad (7)$$

where  $h_{50}$  and  $\pi_{50}$  are the soil-water pressure head and the osmotic head at which the uptake rate is reduced by 50%, respectively, and  $p_1$ , and  $p_2$  are fitting parameters, assumed to be 3 (van Genuchten and Gupta, 1993). Alternatively, if solute effects are not considered, the option is provided to account for pressure head effects only, by using either a simplified form of Eq. (7) or the expression by Feddes et al. (1978) used in Clausnitzer and Hopmans (1994).

Distribution of potential root water uptake sites within the soil domain is lumped into nodal values of a function  $\beta(x, y, z, t)$  [-]. To construct the set of nodal  $\beta$ -values, first the finite element that surrounds each root segment is identified. To each of its eight corner nodes a value is contributed, which is equal to the inverse distance between the center of the segment and the respective corner, and proportional to the segment length. At any time the  $\beta$ -value of a particular node

will increase as the number of active root segments and their respective lengths within its neighboring elements increase, and the distances from the element nodes to the centerpoints of those segments decrease. To account for root-age effects on water uptake (Henriksen et al., 1992; Lazof et al., 1992), piecewise linear weighting functions are defined, which allow for variations in root water uptake for each branch segment depending on age and branching order. Depending on the current value of its weighting factor (between unity and zero), each segment in the root system can fully contribute to, or be partially or totally excluded from uptake.

If solute transport is included in the simulation, root solute uptake is lumped into nodal values of the sink term  $S'(x, y, z, t)$  of Eq. (2):

$$S' = \delta S + (1 - \delta)A \quad (8)$$

where  $\delta$  [-] is a partition coefficient with a value between 0 and 1. The first term of the right-hand side describes passive nutrient uptake ( $S$  is calculated according to Eq. (5)). The second term simulates active nutrient uptake. Experimental results (Kochian and Lucas, 1982; Siddiqi et al., 1990) have shown that the kinetics of active uptake can be described by the sum of a Michaelis-Menten component (Barber, 1984) and a linear component (Kochian and Lucas, 1982):

$$A = \left( \frac{V_{max}}{K_m + c} + f \right) R_d \quad (9)$$

where  $V_{max}$  [ $\text{ML}^{-2}\text{T}^{-1}$ ] is the maximum nutrient uptake rate,  $K_m$  [ $\text{ML}^{-3}$ ] the Michaelis-Menten constant,  $R_d$  [ $\text{L}^2\text{L}^{-3}$ ] the rooting density, and  $f$  [ $\text{LT}^{-1}$ ] is a first-order rate coefficient.

The rooting-density function  $R_d$  is computed at each time step from:

$$R_d(x, y, z, t) = T\sigma'(x, y, z, t) \quad (10)$$

where  $T$  [ $\text{L}^2$ ] is the total root surface area and  $\sigma'$  [ $\text{L}^{-3}$ ] is a function describing the current distribution of potential solute-uptake sites within the domain. The total root surface area  $T$  is obtained from:

$$T = \sum t_i = \sum L_i(2\pi r_i) \quad (11)$$

where  $t_i$  [ $\text{L}^2$ ] is the root segment surface area for each segment  $i$ ,  $L_i$  [ $\text{L}$ ] is the segment length, and  $r_i$  [ $\text{L}$ ] is the segment radius (assumed constant within each segment), calculated from the mass-per-unit-length (as

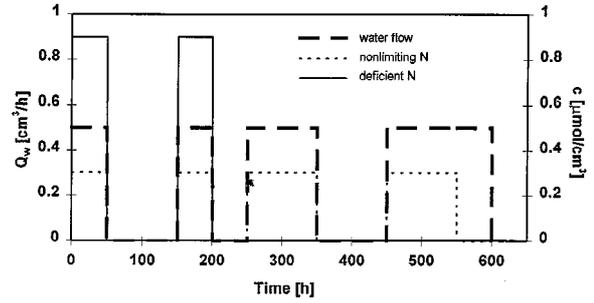


Figure 3. Water and nitrogen application regime for the 'level 2' simulation.

a function of soil strength) and the dry root density, as specified in the input. The function  $\sigma'$  is computed similar to the  $\beta'$  function in Eq. (6), except that nodal values are proportional to the surface area rather than the segment length.

Using a 'level 2' simulation including nutrient transport and uptake ( $\delta = 1$  in Eq. (8)), barley root growth was simulated for a period of 25 days with the irrigation schedule presented in Figure 3. Initial conditions and soil hydraulic, solute-transport and root-growth parameters are presented in Appendix I, while simulation control parameters are presented in Table 2. Soil temperature was assumed to be optimal. In this example, both water and  $\text{NO}_3\text{-N}$  were applied through a dripper, simulated by five nodes at the center of the upper boundary of the simulation domain. A unit-gradient boundary condition was imposed at the domain bottom.

The results in Figure 4 were obtained by supplying the same total amount of  $\text{NO}_3\text{-N}$  ( $225 \mu\text{mol}$ ) in both simulations; however, the distribution in time of the applied fertilizer was different between the two cases (see Fig. 3). The predicted root system and the corresponding uptake intensity ( $\mu\text{mol}/\text{cm}^3\text{h}$ ) of Fig. 4a were obtained by applying  $\text{NO}_3\text{-N}$  with each irrigation event (nonlimiting N). In this case the N supply is sufficient throughout the growth period and the root system presents a regular growth pattern. For the root system and corresponding N-uptake intensity in Figure 4b, N was applied only with the first two irrigation events. For this case, when all the nitrogen enters the domain during the first 200 h of the simulation, much of the applied N moves down and is leached out of the domain before it can be taken up by the roots. Growth is hampered by lack of nutrient supply and roots are sparser, but reach a greater depth driven by the moving  $\text{NO}_3\text{-N}$  plume. Figures 5a and 5b present the cumulative mass balance ( $\mu\text{mol}$ ) for both simulations. The

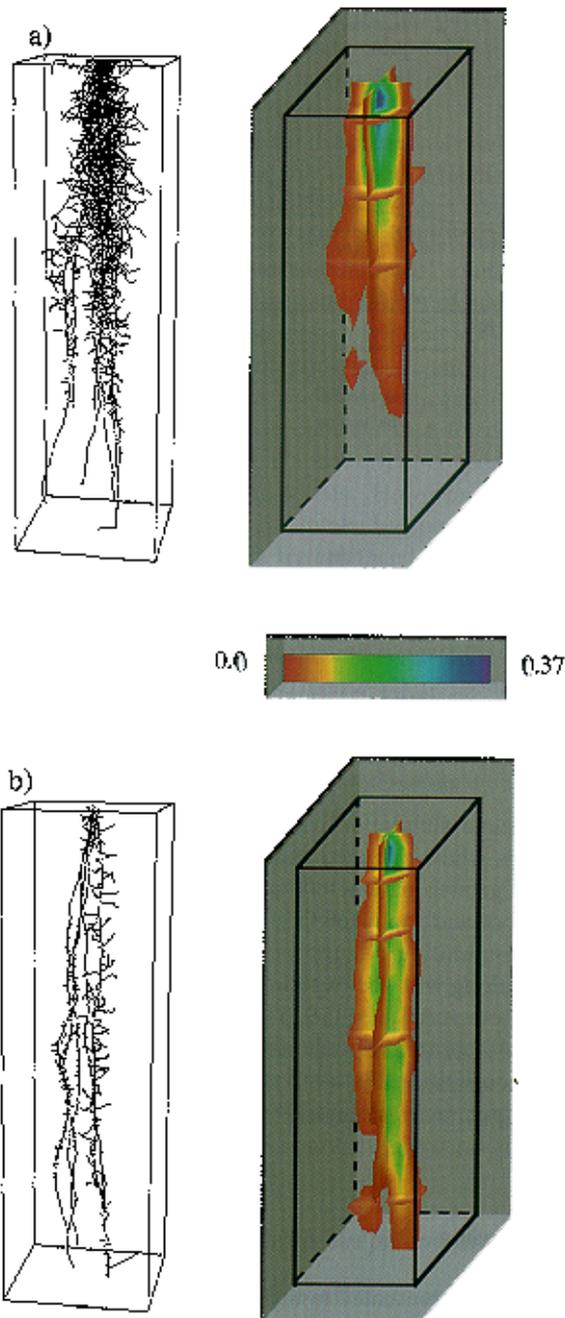


Figure 4. Simulated root system and nutrient uptake rate ( $\mu\text{mol}/\text{cm}^3\text{h}$ ) for: a) sufficient and b) deficient nitrogen supply.

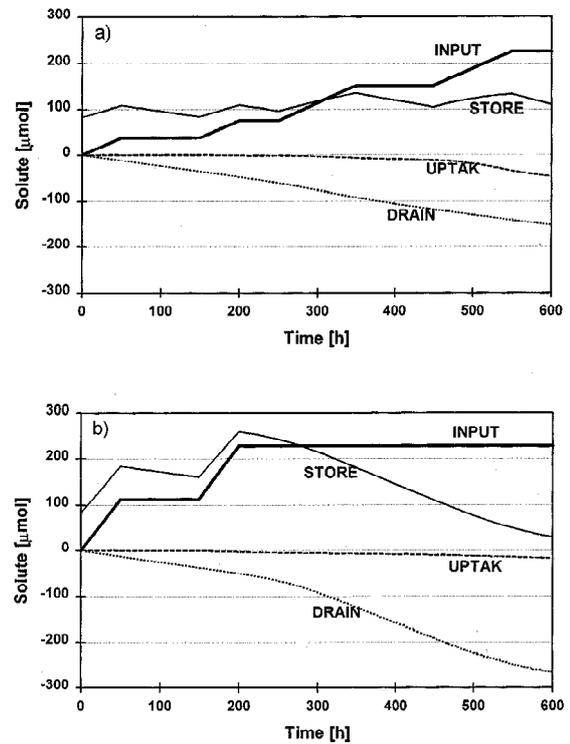


Figure 5. Total amount of N in the domain (STORE), cumulative amount of N entering the domain through the dripper (INPUT), cumulative amount of N removed by the root system (UPTAK), and cumulative amount of N leached (DRAIN) for nonlimiting (a) and deficient (b) N supply.

cumulative mass of N being applied to the root system (INPUT) by the end of growth period (25 days) was identical in both cases. However, for the case of uniformly distributed nitrogen application the mass of N present in the domain (STORE) remained fairly constant (Fig. 5a), while for the deficient N case STORE decreased rapidly after the first two N applications due to leaching (DRAIN) caused by subsequent water applications (Fig. 5b). Consequently, total N uptake (UPTAK) was also significantly lower for the deficient N case (15  $\mu\text{mol}$  versus 50  $\mu\text{mol}$  of the nonlimiting-N case).

#### Shoot and root growth

At the most complex simulation level ('level 3') shoot growth is modeled along with root growth, provided that sufficient information is available to the user. The effects of solute concentration on plant growth can be taken into account if solute transport and root nutrient uptake are included in the simulation.

Potential root and shoot growth is based on four "potential-growth" parameters, each described by a piecewise linear function of time: (1) potential transpiration rate per unit leaf area,  $T_{pot}/LA$ , which allows calculation of potential transpiration as a function of the current leaf area; (2) water-use efficiency,  $W$ , defined as dry mass gained per amount of water transpired; (3) root/shoot allocation ratio of new assimilate  $R$ , which partitions the biomass between the shoot and the roots; and (4) increase in leaf area per incremental increase of new shoot dry mass. The latter parameter is needed to compute the leaf area increment from the amount of biomass allocated to the shoot, and drives plant transpiration.

Biomass allocated to shoot creates increasing leaf area at each simulation time step. However, biomass allocated to roots is accumulated and distributed to roots only during root growth events. At those times, a tentative segment length is calculated for each growing apex as in 'level 1' and '2' simulations, i.e. as a function of the local soil strength, temperature and nutrient concentration conditions. The segment length thus obtained is then adjusted according to the amount of biomass allocated to roots. If the assimilate allocated is smaller than the potential need, the length of all new growing segments is scaled back accordingly. Surplus assimilate is assumed to be exuded by the root system.

In addition to the existing stress factors describing the effects of soil strength on the three plant growth parameters  $T_{pot}/LA$ ,  $W$  and  $R$ , new factors were introduced to account for plant stress due to limiting or toxic solute concentration levels. While the effect of solute concentration on each of these parameters has been described by Schmidhalter and Oertli (1991), Stark (1992), and Ericsson (1995), the combined effects and the interaction with other stress causes (soil strength, water deficiency, and temperature) are still uncertain. To allow complete flexibility in the testing of the relationships between different stresses, and to maintain consistency with the approach adopted by Clausnitzer and Hopmans (1994) for soil strength stress, the above mentioned factors were described by piecewise linear functions of relative stress, the latter in turn being also described by a piecewise linear function of solute concentration. When both soil strength and solute concentration affect the three growth parameters, only the most limiting stress-adjustment factor is used for biomass calculations (Jones et al., 1991).

A 'level 3' simulation was performed for non-limiting N supply and deficient N supply scenarios.

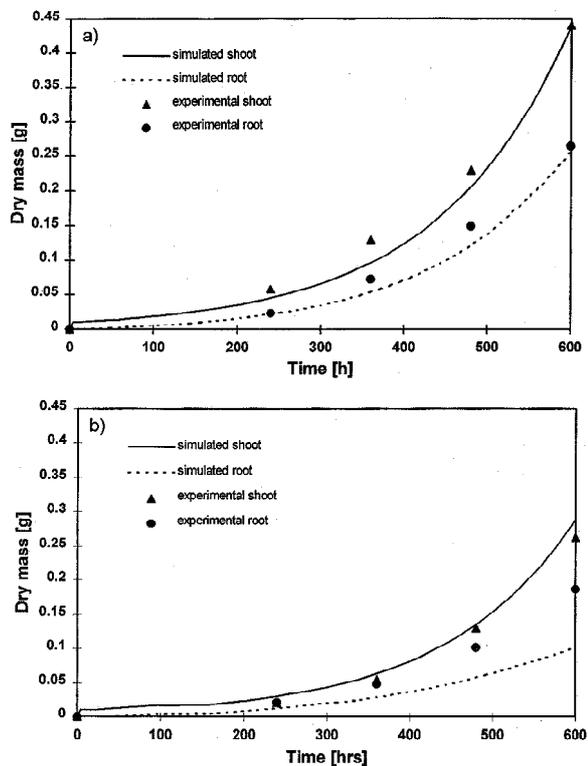


Figure 6. Simulated barley growth curves with: a) nonlimiting nitrogen supply and; b) deficient nitrogen supply. Experimental points indicate data reported by Drew and Saker (1975).

The same simulation parameters and boundary conditions were assumed as in the 'level 1' simulation. Plant growth parameters are presented in Appendix I. Shoot and root growth curves are shown in Figure 6a (nonlimiting N supply) and 6b (deficient N supply), along with the experimental data points reported by Drew and Saker (1975) for barley. Although the model approximates the experimental data better for the nonlimiting N supply than for deficient supply, the agreement between simulation and measurement is satisfactory.

## Conclusion

The model presented in this paper allows the simultaneous, dynamic simulation of root growth and water and solute transport and uptake in three dimensions. Transient root growth processes are simulated by discretizing in time (roots grow at user-defined time steps), and space (at each growth event a new segment is added to each growing root). The length of the segment and its direction are a function of local

soil environmental conditions. Complexity of the soil factors influencing plant transpiration and root growth and uptake can vary depending on the information available to the user. A mechanistic approach, including empirical functions, has been adopted to describe flow and transport and interactions with root and shoot growth.

The intended purpose for the presented model is to provide a tool for studying the interactive relationships between changing soil-water and nutrient status and root activity. Extensions to the Clausnitzer and Hopmans (1994) model include simulation of solute transport and root solute uptake, and effects of additional environmental stresses on root growth and activity, including osmotic potential, nutrient deficiency, and ion toxicity. Root uptake is considered using an empirical macroscopic approach, as opposed to a formulation where local water-potential and nutrient-concentration gradients are the driving forces. However, reduced local water and/or nutrient uptake by root decay and aging is compensated for by enhanced uptake by the remainder of the root system. The authors understand the limitations of the model, including the lack of root competition in its formulation, and suggest that much experimental work is needed to provide the model with the correct parameter values and functional relationships. The flexible structure of the model and easy accessibility of its components should make it a useful workbench for hypothesis testing.

## Appendix I

### Initial conditions

At the beginning of each simulation the soil was at hydraulic equilibrium, with a pressure head of  $-420$  cm at the soil surface. The  $\text{NO}_3\text{-N}$  concentration was  $0.06 \mu\text{mol}/\text{cm}^3$  throughout the soil domain for the examples of Figures 2 and 6, and  $0.1 \mu\text{mol}/\text{cm}^3$  for the example in Figures 4 and 5.

### Soil hydraulic and solute transport parameters

Residual volumetric water content  $\theta_r$  and saturated volumetric water content  $\theta_s$  as well as fitting parameters  $a$  and  $n$ , necessary for the description of the soil water retention and conductivity curves (van Genuchten, 1980) are reported in Table 3. In the same table are also presented the molecular diffusion coefficient  $D_d$  and the longitudinal and transverse dispersivities,  $D_L$  and  $D_T$  respectively, necessary for the

Table 3. Soil hydraulic and solute transport parameters for simulation levels '1', '2' and '3'

Soil hydraulic parameters	Figure			Solute transport parameters	
	1,2	3,4,5	6		
$\theta_r$ :	0	0	0	$\rho[\text{g}/\text{cm}^3]$ :	1.53
$\theta_s$ :	0.55	0.55	0.55	$D_d[\text{cm}^2/\text{h}]$ :	0.0684
$a[\text{cm}^{-1}]$ :	0.003	0.003	0.003	$D_L[\text{cm}]$ :	0.5
$n$ :	3.0	3.0	3.0	$D_T[\text{cm}]$ :	0.1
$K_s [\text{cm}/\text{hr}]$ :	0.75	0.5	0.75		

calculation of the components of the dispersion tensor  $D_{ij}$ , (Šimunek et al., 1992) presented in Eq. (2).

### Root growth parameters

See Table 4.

### Plant growth parameters

The following parameters were used in the 'level 3' simulation presented in Figure 6: Basic (i.e., no stress) plant functions:

- Potential transpiration rate per leaf area:  $0.01 \text{ cm}^3 \text{ H}_2\text{O}/\text{cm}^2 \text{ leaf area}/\text{hr}$
- Water use efficiency:  $0.00535 \text{ g}/\text{cm}^3 \text{ H}_2\text{O}$
- Root/shoot allocation ratio: 0.62

### Soil strength stress factor functions

- Transpiration reduction factor due to relative stress: interpolated between 0.96 at zero stress and 0.625 at relative stress equal to 1.0
- Water use efficiency factor due to relative stress: equal to one at all stress levels
- Root/shoot ratio factor due to relative stress: interpolated between 1 at zero stress and 1.2 at relative stress equal to 1.0

Relative stress defined as a function of soil strength: interpolated between 0 at 1.5 MPa and 1 at 5.3 MPa

### Solute concentration stress factor functions

- Transpiration reduction factor due to relative stress: equal to one for all concentrations
- Water use efficiency factor due to relative stress: interpolated between 1 at zero stress and 0.1 at relative stress equal to 1.0
- Root/shoot ratio factor due to relative stress: interpolated between 1 at relative stress equal to 0.5 and 2 at relative stress equal to 1.0

Table 4. Root growth parameters for simulation levels '1', '2' and '3'.

Parameter	Value
Number of axis in each axis group:	1+2+2+2
Geotropic angle for each axis group (and permitted range of randomness):	-90° (10°) -90° (10°) -90° (10°) -90° (10°)
Weighing factor of the geotropism component of the growth direction vector for axes:	1
Weighing factor of the geotropism component of the growth direction vector for main laterals:	0
Max. branching order:	3
Max. random change in heading angle per root growth time step given for each branching order:	45°, 45°, 45°
Weighing factor of the soil strength gradient:	0.1, 0.5, 0.1
Component of the growth direction vector given for each branching order [cm/MPa]:	0.5
Unimpeded elongation rate given for each branching order [cm/hr]:	0.1, 0.02, 0.008
Soil strength at which root growth ceases [MPa]:	6.0
Max. branch length given for each branching order [cm]:	200, 200, 200
Min. tissue age for subbranch origination given for each, except the highest, branching order [h]:	100, 150
Branching angle given for each, except the highest, branching order:	90°, 90°
Subbranch spacing given for each, except the highest, branching order [cm]:	0.3, 0.3
Ion deficiency/toxicity concentration range [ $\mu\text{mol}/\text{cm}^3$ ]:	0.005, 0.1, 2, 5

Relative stress defined as a function of solute concentration: interpolated between 0 at  $0.5 \mu\text{mol}/\text{cm}^3$  and 1 at  $0 \mu\text{mol}/\text{cm}^3$ .

Leaf area increase per increase in dry shoot mass:  $200 \text{ cm}^2/\text{g}$

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