FUSSIM2

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FUSSIM2

A two-dimensional simulation model for water flow, solute transport, and root uptake of water and nutrients in partly unsaturated porous media

M. Heinen & P. de Willigen

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1 Introduction

Water movement in the root zone supplies the roots with water to fulfill partly or entirely the transpirative demand of the crop. Soil water is the medium for diffusive/dispersive transport of nutrients in the soil. With water nutrients or other solutes are transported towards drains, ditches or (deep) groundwater, or towards the root surface so that nutrient uptake can occur. Moreover, soil biological and soil chemical processes are strongly influenced by water content. Therefore, knowledge of the water content and water movement in the root zone is a prerequisite in soil physical, chemical and biological studies. The governing equation for water movement in porous media is a non-linear partial differential equation. It is non-linear due to the highly non-linear relationships between the important parameters volumetric water content $\theta$, pressure head $h$ and hydraulic conductivity $K$. Only for special relationships between these three parameters analytical solutions can be used. In any other cases numerical solutions of the governing equation must be used. In most studies one-dimensional simulation models are used, i.e. only water movement in the vertical direction is considered. Examples of such models are: DRAINMOD (Skaggs, 1980), SWATRE (Belmans et al., 1983), HYSWASOR (Dirksen et al., 1993). There are several cases of water movement and solute transport that cannot be described by vertical flow/transport only. Examples are water flow and solute transport in drained fields with rapidly changing shallow groundwater levels (De Vos, 1997), water flow and solute transport in drained thin layers of coarse horticultural substrates (Heinen, 1997), or water flow and solute transport in potato ridges (De Willigen et al., 1995). Universal simulation models for multi-dimensional movement of water are scarce. Mostly, multi-dimensional models are set up for a particular problem only. An example of a two-dimensional simulation model is SWMS-2D (now HYDRUS-2D) by Šimunek et al. (1994,1996). At the time SWMS-2D was under development, Heinen (1997) developed a two-dimensional simulation model for the description of water movement, (inert) solute transport and root water and nutrient uptake. In this report we describe the theory of this model and give a description of how to use the model. It is still under development, and it is particularly meant for rectangular flow domains. However, non-rectangular domains can also be considered as was demonstrated by De Willigen et al. (1995) who considered potato ridges, and Heinen (1997) who considered rockwool slabs with a planting cube.

This report is written to describe the theory behind the simulation model. At this time the model is a stand-alone model. It will be incorporated in a large shell model, called FUSSIM, in which coupling of existing models at AB-DLO will occur. For example, coupling of plant growth, water and solute movement plus uptake, and mineralization. The solute part of the model described in this report will be extended to include denitrification and phosphate sorption. Moreover, implementation of drains and mobile-immobile regions are planned.

In Chapter 2 the fundamental theory for water movement, nutrient transport and root water and nutrient uptake is presented. Chapter 3 presents the numerical solution of the water movement and nutrient transport equations. Chapter 4 gives the mathematical descriptions of the hydraulic properties including hysteresis. In Chapter 5 the use of the stand-alone version of the simulation model FUSSIM2 will be described (user’s guide). In Chapter 6 six examples are considered. The first three examples represent a verification for both the water and solute solution procedures, i.e. a comparison between analytical solutions and numerical approximations. These are: 1) linear, transient flow in an unsaturated rectangular flow domain (for two different initial conditions), 2) two-dimensional, non-linear, steady-state flow in unsaturated soil with explicitly known root water uptake (two-dimensional exponential distribution), and 3) transient solute transport under steady-state water conditions consisting of two one-dimensional cases: diffusive transport and dispersive-diffusive transport in a column. The fourth example represents a validation of the simulation model, in which numerically simulated time courses of volumetric water content are compared to measured data, and in which a comparison between simulated and measured breakthrough data is carried out. The fifth example shows that the simulation model can also be used for irregular flow domains, and shows how the simulation data can be used to visualize the flow process. In the sixth example the effect of osmotic potential on root water uptake is considered.
2 Water movement, nutrient transport and root uptake: theory

In this chapter the basic mathematical formulations for water movement and nutrient transport are presented in Sections 2.1 and 2.4, respectively. Boundary and initial conditions for water movement and nutrient transport are discussed in Sections 2.2 and 2.5, respectively, while models for root water and nutrient uptake are given in Sections 2.3 and 2.6, respectively. We assume that the reader is familiar with some basics of soil physics, such as volumetric water content, flux density, porosity, and the head equivalent for soil water potential (see e.g., Hanks & Ashcroft, 1980; Hillel 1980a,b; Koorevaar et al., 1983).

2.1 Water movement in porous media

Water movement in a porous medium always obeys the law of conservation of matter. Mathematically the continuity equation for incompressible water in rigid porous media in three dimensions is written as

\[
\frac{\partial \theta}{\partial t} = - \nabla \cdot (\theta \mathbf{v}) - S_w
\]

where \( \theta \) is the volumetric water content (L\(^3\)L\(^{-3}\)), \( t \) is time (T), \( \nabla \cdot \) is the divergence operator (L\(^{-1}\)), \( \mathbf{v} \) is the velocity (LT\(^{-1}\)) of the water, \( q = \partial \mathbf{v} \) is the volumetric water flux density (L\(^2\)T\(^{-1}\)), and \( S_w \) is the volumetric sink (or source) strength for water (L\(^{-1}\)T\(^{-1}\)), e.g. root water uptake. In general, all dependent variables in this section, such as \( \theta, \mathbf{v}, q \) and \( S_w \), are functions of the independent variables \( x, y, z \) and \( t \), where \( x \) and \( y \) are the horizontal coordinates (L) and \( z \) is the vertical coordinate (L), taken positive downwards. For convenience, the spatial and temporal functional dependency is left out from the notation in this report. For saturated porous media, Darcy (1856) obtained experimentally that \( q \) is proportional to the gradient in water potential. Buckingham (1907) extended Darcy's law to partially saturated porous media. With the water potential expressed as an head equivalent, (the extended) Darcy's law reads

\[
q = -K(\theta) \nabla H,
\]

where \( K \) is the hydraulic conductivity (LT\(^{-1}\)) of the porous medium, \( \nabla \) is the gradient operator (L\(^{-1}\)), and \( H \) is the hydraulic head (L) being the sum of the pressure head \( h \) (L) and the gravitational head \( z_g \) (L):

\[
H = h(\theta) - z_g,
\]

where the minus sign results from \( z \) taken positive downwards. The dependent variables \( K, H \) and \( h \) depend on \( x, y, z \) and \( t \). The relationships \( h(\theta) \) and \( K(h) \) are subject to hysteresis, while \( K(\theta) \) is considered not to be subject to hysteresis (Miller & Miller, 1956); the hydraulic properties are discussed in Chapter 4. The direction of flow is opposite to the gradient in total head, which explains the minus sign in Eq. [2]. Richards (1931) combined Darcy's law and the continuity equation to obtain the governing non-linear partial differential flow equation for water in porous media. For variably saturated, heterogeneous, isotropic, rigid, isothermal porous media and incompressible water (single phase flow), the Richards equation is given by

\[
\frac{\partial \theta(h)}{\partial t} = \nabla \left[ K(\theta) \nabla h(\theta) \right] - \frac{\partial K(\theta)}{\partial z} - S_w.
\]

In unsaturated porous media \( h < h_{cr} \), with \( h_c \) being the air-entry value, and in saturated porous media \( h > h_{cr} \), we assume \( h_{cr} = 0 \). For given relationships between \( K(\theta)h \) (see Chapter 4) and for given initial and boundary conditions (see Section 2.2) and the sink strength (see Section 2.3), the
problem is fully defined and can be solved, provided that flux boundary conditions are not ill-
posed. However, due to the non-linear relationships between \( K \cdot \theta \cdot h \), analytical solutions are
available only for special cases. For most practical problems numerical techniques must be applied, as is done in Chapter 3.

In this report we use the mixed \( \theta \cdot h \) form of the Richards equation (Eq. [4]). In many other studies
the Richards equation is rewritten, so that it has only one dependent variable, either \( \theta \) or \( h \). The
\( \theta \)-based form or diffusivity form of the Richards equation is restricted to unsaturated,
homogeneous porous media and processes not involving hysteresis, and, therefore, not attractive
to be used. The \( h \)-based form of the Richards equation reads

\[
C(h) \frac{\partial h}{\partial t} = \nabla \cdot [ K(h) \nabla h ] - \frac{\partial K(h)}{\partial z} - S_w,
\]

where the differential moisture capacity \( C \) (\( L^{-1} \)) is defined as

\[
C = \frac{d \theta}{d h}.
\]

The \( h \)-based form of the Richards equation can handle partially saturated, heterogeneous porous
media and is used mostly. However, although Eq. [5] is exactly equal to Eq. [4], problems with
respect to mass balance are experienced when solving it numerically. This is not the case when
solving Eq. [4] numerically, as is done in this report (Chapter 3).

It is convenient to introduce here the matric flux potential \( \phi \) (\( L T^{-1} \)) as it will be used later in this
chapter (Gardner, 1958; Raats, 1970):

\[
\phi(h) = \int_{n_{ref}}^{h} K(\eta) \, d\eta,
\]

where \( n_{ref} \) is some reference value for \( h \) and \( \eta \) (\( L \)) is a dummy variable of integration.

### 2.2 Boundary and initial conditions for water movement

The governing flow equation can be solved for given boundary and initial conditions. A general
form of the boundary conditions can be given as (e.g. McCord, 1991)

\[
\mu h + \nu \left. \frac{\partial (h - \eta)}{\partial n} \right|_\Gamma = B,
\]

where \( \mu, \nu \) and \( B \) are given functions evaluated on the boundary \( \Gamma \) of the region which are
dependent on \( x, y, z \) and \( t, n_\Gamma \), is the coordinate normal to \( \Gamma \), and \( \left. \frac{\partial \eta}{\partial n} \right|_\Gamma \) is the exterior normal
derivative operator. The following types are distinguished:

- for \( \mu \neq 0 \) and \( \nu = 0 \), Eq. [8] represents a first-type or Dirichlet boundary condition,
- for \( \mu = 0 \) and \( \nu \neq 0 \), Eq. [8] represents a second-type or Neumann boundary condition, and
- for \( \mu = 0 \) and \( \nu = 0 \), Eq. [8] represents a third-type or Cauchy boundary condition.

In this report we use only the Dirichlet and Neumann conditions.

The Dirichlet condition, with \( \mu = 1, \nu = 0 \) and \( B = h_\Gamma \), in Eq. [8], is given as

\[
h = h_\Gamma,
\]

where \( h_\Gamma \) is the prescribed pressure head at the boundary, e.g. a fixed ground water level at the
bottom represented as \( h = 0 \). Another example is a given \( h \) along the wall of a ditch with a constant
water level.
The Neumann condition, with \( \mu = 0 \), \( \nu = K_f \) and \( B = q_f \) in Eq. [8], is given as

\[
K_f \frac{\partial (h - z)}{\partial n_f} = q_f, \tag{10}
\]

where \( q_f \) is the prescribed volumetric flux density at the boundary, for example, rain or irrigation rates, or no flow across an impermeable boundary. An alternative form of the Neumann condition is the specified hydraulic gradient condition, i.e. with \( \mu = 0 \), \( \nu = 1 \) and \( B = B_f \) in Eq. [8], where \( B_f \) is the specified hydraulic gradient at the boundary. This Neumann condition is given as

\[
\frac{\partial (h - z)}{\partial n_f} = B_f. \tag{11}
\]

Seepage faces

A special type of boundary is a seepage face. Seepage face conditions have been used by e.g. Rubin (1968), Neuman et al. (1974), Cooley (1983) and Simunek et al. (1994,1996). In case the porous medium is saturated at the seepage face there will be outflow and the boundary condition will be of Dirichlet type, i.e. \( h_f = 0 \). As soon as the porous medium at the seepage face becomes unsaturated, the boundary condition will be that of no-flow Neumann type, i.e. \( q_f = 0 \). The seepage face may be partly of Neumann type and partly of Dirichlet type. Heinen (1997) used a seepage face condition to represent a free outflow drain at the bottom of his sand bed system. The seepage face conditions at the boundary are determined as follows (Dirichlet)

\[
\text{for } q_f \geq 0, \quad h_f = 0, \tag{12}
\]

or (Neumann)

\[
\text{for } h_f < 0, \quad q_f = 0. \tag{13}
\]

Unit H-gradient bottom boundary condition

A special case of the specified hydraulic gradient at the bottom boundary is the unit H-gradient outflow condition (cf. Eq. [10]). The value of the specified flux across the boundary then equals the value of the local hydraulic conductivity, according to

\[
K_f = q_f. \tag{14}
\]

Such a condition can be useful as a bottom boundary condition when the water table lies far below the domain of interest (e.g. McCord, 1991).

A resistance drain

A special drain condition is the so-called resistance drain condition. Water outflow into the drain occurs at a flux density equal to the difference in pressure head in the soil and that in the drain \( h_d \) (usually zero) divided by the drain resistance \( r_d (T) \) according to

\[
\text{if } h > h_d, \quad \frac{h - h_d}{r_d} = q_f, \tag{15}
\]

or

\[
\text{if } h \leq h_d, \quad 0 = q_f. \tag{16}
\]

Resistance drains can be present at the bottom of the soil profile.

Initial condition

In order to start computations with the numerical simulation model (as described in Chapter 3) an initial condition of the system has to be supplied. The initial condition is given as an initial pressure head \( h_0 \) distribution.
At all positions $h$ is given and related quantities such as $\theta$ and $K$ (see Chapter 4) can be computed.

2.3 Root water uptake

Consider one layer of substrate of thickness $\Delta z$ (L) with equally distributed, parallel roots perpendicular to the porous medium surface. Each root with a radius of $R_r$ (L) is surrounded by a part of the substrate which can be represented by an equivalent hollow cylinder. The outer radius of this equivalent hollow cylinder $R_1$ is simply related to the root length density $L_r$ (L$^{-3}$), i.e. root length per unit volume of porous medium, according to

$$R_1 = \left(\frac{1}{\sqrt{\pi L_r}}\right)^{-1}. \quad [18]$$

De Willigen & Van Noordwijk (1987) developed a microscopic model for root water uptake. For one root surrounded by a hollow cylinder of substrate, the rate $q_i$ (L$^{-3}$) of water movement from the substrate towards the root surface is equal to the uptake rate $q_i$ (L$^{-3}$) by the root, which in turn is equal to the actual transpiration rate $T$ (L$^{-3}$):

$$q_1 = q_2 = T. \quad [19]$$

In this analysis the amount of water needed for growth and turgor regulation is disregarded. A schematic representation of the geometry and notation convention for root water uptake is given in Fig. 1.

![Figure 1](image_url) Geometry and notation convention root water uptake model: (A) horizontal and (B) vertical cross sections through root and substrate cylinder.
Now it is possible to extend the single root model to a layer with known root length density. Within $\Delta z$ there is supposed to be no vertical gradient in $h$, so that only radial flow towards the root surface is considered. In what follows, expressions for the three terms of Eq. [18] will be given. We do not use vector notation for fluxes to or away from individual roots, but only the magnitudes of the fluxes, with flow towards or into the root being positive.

The uptake rate $q_1$, by roots from one layer of thickness $\Delta z$ with a given root length density $L_r$, is given as (see also e.g. Dalton et al., 1975)

$$q_1 = \Delta z L_r K_1 (h_{rs} - h_r + \sigma_r (h_{os} - h_{or})), \tag{20}$$

where $K_1$ is the root hydraulic conductance (LT$^{-1}$), $h_r$ is the root pressure head assumed to be uniform over the whole root system, $h_{rs}$ is the pressure head at the root-substrate interface, $\sigma_r$ is the reflection coefficient for solutes at the root membrane with $\sigma_r \in [0,1]$ (1), $h_{os}$, $h_{or}$, is the osmotic potential (L) at the root-substrate interface (see at the end of Section 2.4), and $h_{or}$ is the osmotic potential of the root system assumed to be uniform over the whole root system. The variables $q_1$, $L_r$, $h_r$, $h_{rs}$, $h_{os}$, and $h_{or}$ are generally time-dependent. In principle, $K_1$ can be dependent on $h_r$, and $t$, but this is not considered in this report, i.e. $K_1$ is assumed to be constant (see also discussion in De Willigen & Van Noordwijk, 1987). By setting $\sigma_r = 0$ the effect of osmotic pressure head $h_o$ on water uptake is disregarded.

Due to the highly non-linear relationship in the hydraulic properties, it is not possible to obtain an analytical solution for water movement in the substrate around the root. However, De Willigen & Van Noordwijk (1987) showed that a steady-rate solution for the matric flux potential (Eq. [7]) distribution $\phi(R)$ (L$^2$T$^{-1}$) can be used for a certain uptake rate $q_2$ given by

$$\phi(R) = \phi(R_0) + \frac{q_2}{2 \pi L_r \Delta z} \left( \rho^2 \ln \frac{R}{R_0} - \frac{(R/R_0)^2 - 1}{2(\rho^2 - 1)} \right), \tag{21}$$

where $R$ is the radial coordinate (L), and $\rho$ is a dimensionless reduced radius of the substrate cylinder surrounding each root defined by $\rho = R/R_o$.

From Eq. [21] it follows that the rate $q_2$, at which water arrives at the root surface is proportional to the difference between the average matric flux potential in the hollow soil cylinder surrounding the root $\bar{\phi}$ and the matric flux potential $\phi_r$ at the soil/root interface (De Willigen, 1990):

$$q_2 = \Delta z \pi L_r \frac{(\rho^2 - 1)}{G_o(\rho)} (\bar{\phi} - \phi_r), \tag{22}$$

with $\bar{\phi}$ defined as

$$\bar{\phi} = \frac{\int_{R_0}^{R_1} 2R \phi(R) dR}{R_1^2 - R_0^2}, \tag{23}$$

and $G_o(\rho)$ is a dimensionless geometry function given by

$$G_o(\rho) = \frac{1}{2} \left( \frac{1 + 3\rho^2}{4} + \frac{\rho^4 \ln \rho}{\rho^2 - 1} \right), \tag{24}$$

$G_o(\rho)$ is a special case of the geometry function $G(\rho,\sigma)$ given in Section 2.6 (Eq. [51]).

The actual transpiration rate $T$ can be assumed to be a function of the potential transpiration rate $T_p$ (LT$^{-1}$) and the root water pressure head $h_r$ according to
\[ T = f_r(h_r) T_p. \] \[ \text{[25]} \]

For example, Campbell (1985, 1991) gave the following reduction function (Fig. 2)

\[ f_r(h_r) = \left[ 1 + \left( \frac{h_r}{h_{r,1/2}} \right)^a \right]^{-1}, \] \[ \text{[26]} \]

where \( h_{r,1/2} \) is a species-dependent plant pressure head at which, \( T = 0.5T_p \) and \( a \) is a species-dependent dimensionless constant.

The root water uptake model is solved by finding \( h, h_r, \) and \( T \) for given pressure head in the substrate so that Eq. [18], with Eqs. [20], [22] and [25]+[26], is satisfied. It is assumed that \( \sigma, h_{en}, \) and \( h_{en} \) are explicitly known; \( h_{en} \) follows from the electrical conductivity near the root as described at the end of Section 2.4. Due to the non-linear relationships between \( h \) and \( \phi \) and between \( T \) and \( h_r \), the solution has to be found iteratively. The root water uptake can be used as the sink strength \( S_w \). Here the single root model was extended to a single layer with given root length density. It can be extended to multi-layers or to compartments, each with its own root length density (see Subsection 3.2.5).

The \( \phi(h) \) relationship is hysteretic, and the root water uptake module should account for that. Explicit formulations for \( K(h) \) scanning curves are not available to our knowledge. Principally, one could derive these scanning curves from the \( \phi(h) \) and \( K(\theta) \) relationships. This needs further research and is not included in this report. Both \( \phi_h \) and \( \phi_u \) will be obtained from the main drying \( K(h) \) relationship, and thus will be overestimated. As long as the difference between \( h \) of the bulk soil in the hollow soil cylinder and \( h_r \) is not too large, it is anticipated that the error in disregarding hysteresis will be small. Such situations can be expected under wet conditions.

**Figure 2** The transpiration reduction function, Eq. [26], as a function of the root pressure head for three sets of parameter values \( h_{r,1/2} \) and \( a \).
Under very wet conditions, e.g. in greenhouse substrates, the steady-rate solution for water distribution around a root can also be expressed in terms of volumetric water content according to

\[
\theta(R) = \theta(R_0) + \frac{T}{2 \pi \Delta z L_{rv}} D_w \left[ \frac{\rho^2}{\rho^2 - 1} \ln \frac{R}{R_0} - \frac{(R/R_0)^2 - 1}{2(\rho^2 - 1)} \right].
\]  

[27]

Note that Eq. [27] is similar to Eq. [21], except for the presence of the diffusivity \(D_w\) (L^2·T^{-1}). Under these wet conditions the gradient in \(\theta\) may be very small or negligible, so that \(h_n = h\) and thus \(\overline{\phi} = \phi_{nr}\). In that case in Eq. [26] \(h_n\) can be replaced by \(h\), and the solution of the water uptake model is restricted to finding \(q_s\) and \(h\), without considering Eq. [22]. In case no transpiration reduction occurs, \(h\), can be computed from

\[
h_r = h - \frac{T}{K_i L_{rv} \Delta z} - \sigma_s (h_{s,fs} - h_{s,fr}).
\]

[28]

2.4 Nutrient transport in porous media

The continuity or mass balance equation for nutrient transport at any point in a rigid porous medium is given by (e.g. Bolt, 1982)

\[
\frac{\partial Q}{\partial t} = -\nabla \cdot q_s - S_s,
\]

[29]

where \(Q\) is the total density (ML^{-3}) of the nutrient present in the porous medium, \(q_s\) is the nutrient mass flux density (ML^{-2}·T^{-1}), and \(S_s\) is a mass sink (or source) strength (ML^{-2}·T^{-1}) for a solute or nutrient, e.g. root nutrient uptake. In general, all dependent variables in this section are dependent on \(x, y, z\) and \(t\). Equation [29] must be used for each nutrient separately. The nutrient can be present in solution, at the adsorption complex, or as a precipitate. In this report we assume that precipitation does not occur and that the porous medium is inert, i.e. it has no adsorption complex for all nutrients present, so that \(Q\) is given as

\[
Q = \theta c,
\]

[30]

where \(c\) is the nutrient concentration (ML^{-3}). Nutrient transport is by mass flow with the water and by diffusion and dispersion due to gradients in concentration, so that \(q_s\) is given as

\[
q_s = q c - D_h \cdot \nabla c,
\]

[31]

where \(D_h\) is the hydrodynamic dispersion tensor (L^2·T^{-1}) being the sum of the dispersion and diffusion tensors. It is symmetric for isotropic porous media. Using Eqs. [30] and [31], Eq. [29] can be written as

\[
\frac{\partial \theta c}{\partial t} = -\frac{\partial q_i c}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \theta D_{ii} \frac{\partial c}{\partial x_j} \right) - S_s, \quad i, j = 1, 2, 3,
\]

[32]

where subscripts \(i\) and \(j\) refer to the three perpendicular coordinate axes. The expression for \(D_{ij}\) for partially saturated porous media is given by Bear & Verrrujst (1987) and Simunek et al. (1994,1996) as

\[
\theta D_{ij} = a_l |q| \delta_{ij} + (a_t - a_l) \frac{q_i q_j}{|q|} + \theta D_o \tau(\theta) \delta_{ij},
\]

[33]

where \(a_l\) and \(a_t\) are the longitudinal - along a streamline - and transversal - perpendicular to a streamline - dispersivities (L), respectively, \(|q|\) represents the absolute magnitude of \(q\) (LT^{-1}), \(\delta_{ij}\) is the Kronecker delta function with \(\delta_{ij} = 1\) when \(i = j\) and \(\delta_{ij} = 0\) when \(i \neq j\), \(D_o\) is the molecular diffusion
coefficient in free water (LT⁻¹; see description below), and \( \tau \) is the tortuosity factor (1) which accounts for the increased path length in porous media, which is a function of \( \theta \). We use the broken-line \( \tau(\theta) \) relationship from Barraclough & Tinker (1981; their Fig. 1) given by

\[
\tau(\theta) = \begin{cases} 
  f_1 \theta + f_2 & \theta \geq \theta_1 \\
  \theta(f_1 \theta_1 + f_2) / \theta_1 & \theta < \theta_1 
\end{cases}
\]  

[34]

where \( f_1, f_2 \) and \( \theta_1 \) are dimensionless parameters. Barraclough & Tinker (1981) obtained two sets of data, one for clay soils, and one for sand and loamy soils, for which the parameters occurring in Eq. [34] were determined (Table 1).

According to Bear & Verruijt (1987) \( \alpha_1 \) is 10 to 20 times larger than \( \alpha_r \), in one-dimensional studies only one dispersivity is determined. For example, Beven et al. (1993; their Table 5) summarized values measured in partially saturated undisturbed field core samples or plots, ranging from 0.0087 m to 1.116 m.

The governing nutrient transport equation can be solved for all nutrients present in the solution. Currently, the model can handle the nutrients N (NO₃ and/or NH₄), K, P, Ca, Mg, S, Cl, and Na.

Table 1  Values for the dimensionless parameters \( \theta_1, f_1 \) and \( f_2 \) occurring in Eq. [34] derived from data of Barraclough & Tinker (1981; their Fig. 1).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Sand or loam</th>
<th>Clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_1 )</td>
<td>0.12</td>
<td>0.20</td>
</tr>
<tr>
<td>( f_1 )</td>
<td>1.58</td>
<td>0.99</td>
</tr>
<tr>
<td>( f_2 )</td>
<td>-0.17</td>
<td>-0.17</td>
</tr>
</tbody>
</table>

**Electrical conductivity**

According to the theory of ionic mobilities and ionic conductance in electrolyte solutions the electrical conductivity \( \text{EC} \) of a solution can be given as a function of the concentration (Atkins, 1978; Bard & Faulkner, 1980; Chang, 1981). In fact activities instead of concentrations should be used (Kamphorst & Bolt, 1981). In that case \( \text{EC} \) (dS m⁻¹) is given by (see also Heinen, 1990, 1997)

\[
\text{EC} = F \sum_{i=1}^{m_s} \rho_i c_i n_{i,j} \mu_{m,i} f_{a,i} 
\]  

[35]

where \( F \) is Faraday's constant (96485 C mol⁻¹), \( m_s \) is the number of solutes, \( \rho_i \) is the density of the solvent (kg dm⁻³), \( c_i \) is the concentration of ion \( i \) (mol kg⁻³), \( n_{i,j} \) is the absolute valence of ion \( i \) (-), \( \mu_{m,i} \) is the ionic mobility of ion \( i \) (cm² s⁻¹ V⁻¹); Table 2), and \( f_{a,i} \) is the activity coefficient of ion \( i \) (-). The activity coefficient \( f_{a,i} \) depends on the total concentration, i.e. ionic strength \( I_s \) (mol kg⁻³) of the solution, where \( I_s \) is defined as

\[
I_s = 0.5 \sum_{i=1}^{m_s} c_i n_{i,j}^2 
\]  

[36]

This dependence \( f_{a,i}(I_s) \) is described by the extended Debye-Hückel theory according to (Atkins, 1978; Chang, 1981; Novozamsky et al., 1981).
\[
    \log f_{o,i} = -\frac{A_f n_{o,i}^2 \sqrt{I_s}}{1 + B_f d_{i,j} \sqrt{I_s}},
\]

with (Atkins, 1978)

\[
    A_f = \frac{N_o e^3 \sqrt{2 \rho_s}}{8 \pi (\varepsilon_o \varepsilon_r R_g T)^{1.5} \ln 10},
\]

and

\[
    B_f = \frac{N_o e \sqrt{2 \rho_s}}{(\varepsilon_o \varepsilon_r R_g T)^{0.5}},
\]

where \(d_i\) is the effective diameter of the ion (m; Table 2), \(N_o\) is Avogadro's number (= 6.022 \times 10^{23} \text{ mol}^{-1}), \(e\) is the electron charge (= 1.6022 \times 10^{-19} \text{ C}), \(\varepsilon_o\) is the dielectric permittivity of vacuum (= 8.8542 \times 10^{-12} \text{ C}^2 \text{ V}^{-1} \text{ m}^{-1}), \(\varepsilon_r\) is the relative dielectric permittivity of the solvent, \(R_g\) is the universal gas constant (= 8.3144 \text{ J} \text{ mol}^{-1} \text{ K}^{-1}), and \(T\) is the temperature (K). The Debye-Hückel theory assumes that the electrolytes are completely dissociated into ions in solution and that each ion is surrounded by ions of opposite charge. For \(T = 298\text{ K}\) and water as solvent (\(\varepsilon_r = 78.54\), \(\rho = 1000\text{ kg m}^{-3}\)) the parameters \(A_f\) and \(B_f\) become \(A_f = 0.51\) (mol kg\(^{-1}\))\(^{0.5}\) and \(B_f = 3.3 \times 10^9\) (mol kg\(^{-1}\))\(^{0.5}\) m\(^{-1}\). For very dilute solution \(I < 0.005\text{ mol kg}^{-1}\) according to Bates (1978); \(I < 0.01\text{ mol kg}^{-1}\) according to Chang (1981) or when ions are assumed to be points, i.e. \(d_i = 0\), one obtains the limiting Debye-Hückel law:

\[
    \log f_{o,i} = -A_f n_{o,i}^2 \sqrt{I_s}.
\]

In case \(d_i\) is assumed to be \(d_i = 3 \times 10^{-10}\text{ m}\) and equal for all ions in the solution, the Debye-Hückel law becomes (Günterberg approximation) \((B_f = 3.3 \times 10^9\text{ mol kg}^{-1}\)^{0.5}\text{ m}^{-1}; \text{cf. Eq. \([37]\)})

\[
    \log f_{o,i} = -A_f n_{o,i}^2 \sqrt{I_s}.
\]

For high values of \(I_s\), say \(I_s > 0.1\text{ mol kg}^{-1}\), one can use the Davies extension (Bates, 1978):

\[
    \log f_{o,i} = -A_f n_{o,i}^2 \sqrt{I_s} + 0.1 n_{o,i}^2 I_s.
\]

As a rough approximation EC (dS m\(^{-1}\)) is equal to the sum of the concentration of all ions (in mmol l\(^{-1}\) !!!) divided by 10, where this factor 10 follows from \(10^5 F^2 n_i \mu_m \text{ with } f_{o,i} n_i \text{ and } \mu_m\) representing some average values for \(f_{o,i}\) (say 0.9), \(n_i\) (say 1.5) and \(\mu_m\) (say \(7.5 \times 10^{-4}\text{ cm}^2\text{ s}^{-1}\text{ V}^{-1}\)), respectively, and \(10^5\) is the correction for mmol to mol.

**Diffusion coefficient in free water \(D_0\)**

For each nutrient a diffusion coefficient \(D_0\) is needed. For an ideal solution it can be computed from the ionic mobility \(\mu_m\) (L² T⁻¹ V⁻¹) according to (Atkins, 1978)

\[
    D_0 = \frac{\mu_m k_b T}{n_i e},
\]

where \(k_b\) is the Boltzmann constant (= 1.381 \times 10^{-23} \text{ J} \text{ K}^{-1}). The values for \(D_0\) for all nutrients are listed in Table 2.
Table 2  Values for ionic mobility \( \mu_m \) (10^4 cm^2 s^-1 V^-1); from Chang, 1981 or Bard & Faulkner, 1980), ion diameter \( d_i \) (10^-6 m); from Novozamsky et al., 1981), and diffusion coefficient in free water \( D_o \) (cm^2 d^-1) for several ions commonly present in nutrient solutions.

<table>
<thead>
<tr>
<th></th>
<th>NO_3</th>
<th>H_3PO_4</th>
<th>SO_4</th>
<th>Cl</th>
<th>NH_4</th>
<th>K</th>
<th>Ca</th>
<th>Mg</th>
<th>Na</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu_m )</td>
<td>7.40</td>
<td>7.84(^1)</td>
<td>8.27</td>
<td>7.91</td>
<td>7.61</td>
<td>7.62</td>
<td>6.16</td>
<td>5.50</td>
<td>5.19</td>
</tr>
<tr>
<td>( d_i )</td>
<td>3.0</td>
<td>4.0</td>
<td>4.0</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
<td>6.0</td>
<td>8.0</td>
<td>4.0</td>
</tr>
<tr>
<td>( D_o )</td>
<td>1.64</td>
<td>1.74</td>
<td>0.92</td>
<td>1.76</td>
<td>1.69</td>
<td>1.69</td>
<td>0.685</td>
<td>0.61</td>
<td>1.15</td>
</tr>
</tbody>
</table>

\(^1\) since no value is known it is set equal to the average of the values for NO_3 and SO_4

Osmotic pressure head \( h_o \)

The osmotic pressure head \( h_o \) as used in the root water uptake model (Section 2.3), is due to the presence of solutes in the water. It can be estimated from the EC according to (US Salinity Laboratory Staff, 1954)

\[
    h_o = -400 \, EC ,
\]

where the factor 400 is a conversion factor with dimension cm m dS^-1, so that \( h_o \) is obtained with units cm.

2.5  Boundary and initial conditions for nutrient transport

In general, the boundary conditions for nutrient transport can be of the same type as those for water movement (see Section 2.2), i.e. Dirichlet and Neumann conditions. An example for a Dirichlet condition, \( c_n \), is a constant concentration in a ditch. Rain or irrigation water containing a solute leads to a Neumann condition. Currently, the model assumes that the solute flux density condition is given as the product of the water flux density times a concentration. Thus, a flux density boundary condition is supplied by a concentration value. The water flux density is that used in the water computations.

The initial condition is that of given initial concentration \( c_o \) distribution

\[
    c_t \big|_{t = 0} = c_o(x,y,z) ,
\]

or that of given amount \( Q_{m0} \) (M)

\[
    Q_{m} \big|_{t = 0} = Q_{m0}(x,y,z) .
\]

The amount \( Q_m \) and the density \( Q \) are related according to

\[
    Q = Q_m \, V ,
\]

where \( V = \Delta x \Delta y \Delta z \) is the volume (L^3) of the porous medium.

2.6  Root nutrient uptake

De Willigen & Van Noordwijk (1987, 1994a,b) developed a microscopic model for nutrient uptake. Like for root water uptake, one can consider a layer of substrate of thickness \( \Delta z \) with equally distributed, parallel roots perpendicular to the porous medium surface, i.e. with uniform root length density \( L_m \). Root nutrient uptake is assumed to be primarily dictated by the requirement of the plant, denoted as \( S_p \) (ML^-3 T^-1). Required uptake cannot occur when the diffusion and mass flow processes in the substrate cannot resupply enough nutrient to the root. It is then assumed that the uptake rate equals the maximum possible rate of transport to the root, i.e. the root behaves as a
zero sink. De Willigen & Van Noordwijk (1994b) obtained a steady-rate approximate solution for the concentration profile around the root for the zero-sink condition given as

$$c(R) = -\frac{S_{st}}{2\pi \Delta z L_r D} \left( \frac{R^{2\sigma + 2} - R^{2\sigma}}{2(\rho^{2\sigma + 2} - 1)} + \frac{\rho^{2\sigma + 2}(1 - R^{2\sigma})}{2(\rho^{2\sigma + 2} - 1)} \right),$$  \[48\]

where $D$ is the diffusion coefficient ($L^2 T^{-1}$), and $\sigma$ is the dimensionless water uptake by the root defined as

$$\sigma = -\frac{q_s}{4\Delta z \pi L_r D}.$$  \[49\]

Note that no dispersion coefficient is included above. Since it is expected that only small water fluxes occur, it is neglected.

If the approximate concentration distribution given in Eq. [48] holds, it can be derived that the maximum possible nutrient uptake rate per unit surface area of substrate $S_{sm}$ ($ML^{-2}T^{-1}$) is given as

$$S_{sm} = \pi \Delta z L_r D \bar{c} \frac{\rho^2 - 1}{G(\rho, \sigma)}.$$  \[50\]

where $\bar{c}$ is the average bulk concentration in the substrate layer, and the dimensionless geometry function $G$ is given by (De Willigen & Van Noordwijk, 1994a,b) \(^1\) (Fig. 3)

$$G(\rho, \sigma) = \frac{1}{2(\sigma + 1)} \left( 1 - \frac{1 - \rho^2}{2} + \frac{\rho^2(\rho^{2\sigma} - 1)}{2\sigma} + \frac{\rho^2(\rho^{2\sigma} - 1)(\sigma + 1)}{2(\rho^{2\sigma + 2} - 1)} \right)$$  \[51\]

where in the limit $\sigma \to 0$, i.e. transport is by diffusion only, Eq. [51] reduces to Eq. [24] (Section 2.3).

The actual uptake rate to be used as the sink strength $S_s$ in Eq. [29] is equal to the minimum of the required uptake rate and the maximum uptake rate according to

$$S_s = \min \left( S_{st}, \frac{S_{sm}}{\Delta z} \right).$$  \[52\]

As for root water uptake, this approach can be extended to multi-layered porous media or media with compartments of uniform root length density (see Subsection 3.4.3).

Nutrient transport can be easily extended to include adsorption and/or precipitation, i.e. these amounts have to be included in $Q$. The root uptake models developed by De Willigen & Van Noordwijk (1987, 1994a,b) are based on approximate steady-rate solutions. These authors showed that these approximations were very close to available analytical or numerical solutions for ranges of the parameter values they used. These models are based on regular root distributions. It is known that actual root distributions are non-regular and sometimes even clustered, and that partial root-substrate contact exists. De Willigen & Van Noordwijk (1987) showed that the actual uptake under these conditions is lower than the uptake based on regular root distribution assumptions. Lower uptake due to non-uniformity and clustering of root distributions was also concluded by Rappoldt (1992) based on a different approach. For simplicity reasons, however, we decided to use the simple model.

\(^1\) The expression given by De Willigen & Van Noordwijk (1987; Eq. 9.29, p. 130) is incorrect.
The geometry function $G$ as a function of the reduced radius $\rho$ according to Eq. [51] for five values of $\sigma$, i.e. 0, -0.001, -0.005, -0.01, -0.02; for $D = 0.1 \text{ cm}^2\text{d}^{-1}$ (De Willigen & Van Noordwijk, 1987), $\Delta z = 10 \text{ cm}$, and $L_n = 2 \text{ cm cm}^{-2}$; this corresponds to water uptake of 0, 0.025, 0.126, 0.25 and 0.50 cm d$^{-1}$, respectively.
3 Water movement, nutrient transport and root uptake: numerical implementation

As mentioned in Chapter 2, the Richards equation has to be solved numerically in most cases. In this chapter the Richards equation is implicitly solved, using one of the possible numerical procedures, in this case a sub-domain finite element method (Sections 3.1-3.3), where root water uptake is treated explicitly. The nutrient transport equation is explicitly solved in Section 3.4, making use of the new status of the water and explicitly known root nutrient uptake. In Section 3.5 the time-stepping procedure is described. For convenience, the functional dependence of the dependent variables is left out of the notation.

3.1 Introduction

In general, numerical methods can be divided into discrete domain methods, boundary methods and integral domain methods (Nieber & Feddes, 1996). They can be fully explicit, fully implicit, or a mixture of explicit and implicit such as the Crank-Nicholson method.

A classical example of a discrete domain method is the finite difference method using the Taylor expansion series. The finite difference method is mathematically simple, but rather inflexible, and difficult to use in treating boundary conditions and in coping with irregular boundaries.

The boundary methods seek a solution on the boundary of the solution domain. Only the boundary to be considered and not the interior of the domain. Once the solution at the boundary is obtained, it is possible to obtain at selected interior points values of the dependent variable. It is favoured when the main interest is at the boundary of the solution domain, e.g. Pullan & Collins (1987) used it to determine the effectively wetted region from infiltration from buried and surface cavities.

An example of an integral domain method is the finite element method. This method is physically correct due to the integral approach, but mathematically complex. Moreover, irregular flow domains and boundary conditions can be treated easily. In finite elements usually the method of weighted residuals is applied among which the Galerkin method (e.g. Simunek et al., 1994, 1996) and subdomain method (Cooley, 1983) are well known. The first is mathematically more complex to handle than the second. A special case of the subdomain method is the Control Volume (CV) method with rectangular subdomains, which as applied in heat and fluid flow problems by Patankar (1980), Meurs (1985) and Heinen (1997). The CV method is easy to understand and lends itself to direct physical interpretation. The CV approximated equations are similar to finite difference equations. A method which results in similar numerical equations is the integrated finite difference method as described by Narasimhan & Witherspoon (1976, 1977) and Narasimhan et al. (1977). However, unlike the CV method the integrated finite difference method still needs auxiliary nodes to handle boundary conditions. In the following the CV method will be used.

There are several cases of water movement and solute transport that cannot be described by vertical flow/transport only (see Chapter 1, Introduction). In several cases due to symmetry reasons the actual flow and transport can be considered in two dimensions. In what follows we will use the two-dimensional ($x, z$) form of the mixed $\theta-h$ Richards equation, Eq. [4], written as

$$\frac{\partial}{\partial x} \left( K \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial z} \left( K \frac{\partial h}{\partial z} \right) - \frac{\partial K}{\partial z} - S_w - \frac{\partial \theta}{\partial t} = 0.$$  [53]
3.2 The control volume method

In Subsection 3.2.1 a brief description of the method of weighted residuals is given. The control volume geometry is described in Subsection 3.2.2. The integration of the Richards equation and the boundary conditions are described in Subsections 3.2.3 and 3.2.4, respectively. In Subsection 3.2.5 the solution for root water uptake is presented. The description of the CV method is based on the work of Patankar (1980).

3.2.1 Method of weighted residuals

The method of weighted residuals can be briefly described as follows. Let a differential equation, e.g. Eq. [53] rewritten in h-based form, be represented by

$$\mathcal{L}(h) = 0,$$  \hspace{1cm} [54]

where \(\mathcal{L}\) is some differential operator. Assume a simple approximate solution \(h^*\) that contains a number of undetermined parameters. The substitution of \(h^*\) in the differential equation leaves a residual \(r\) defined as

$$r = \mathcal{L}(h^*).$$  \hspace{1cm} [55]

The best solution is obtained when \(r\) is as small as possible over the whole region. It is proposed that the residual is distributed according to

$$\int_V wr \, dV = 0,$$  \hspace{1cm} [56]

where \(w\) is a weighing function, which is a function of space only, and \(V\) represents the complete flow domain under study. By choosing a succession of \(w\) values one can generate as many equations as needed for evaluating the parameters in \(h^*\). In fact, a number of subdomains are chosen in \(V\) for each of which the Eq. [56] is set up. Different weighing functions \(w\) can be chosen. In the subdomain method the weighing function has the form \(w = 1\) or \(w = 0\). A number of weighted-residual equations can be generated by dividing \(V\) into subdomains further called Control Volumes (CV) and setting \(w = 1\) within each CV and \(w = 0\) everywhere else in \(V\). Thus, integration over \(V\) as in Eq. [56] now becomes integration over the volume \(CV\) of the control volume. Using Eq. [53] and \(w = 1\), and leaving out the superscript * for convenience, this yields

$$\int_{CV} \left[ \frac{\partial}{\partial x} \left( K \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial z} \left( K \frac{\partial h}{\partial z} \right) - \frac{\partial K}{\partial z} - S_w - \frac{\partial \theta}{\partial t} \right] \, dCV = 0,$$  \hspace{1cm} [57]

where \(CV\) (L^3) is the volume of a CV. From now on, the dependent variables refer to the as yet unknown approximated numerical solution. The most attractive feature of the CV method formulation is that the resulting solution would imply that the integral conservation of mass is exactly satisfied over each CV, any group of CV's and over the whole calculation domain.

3.2.2 Control volume geometry

There are several ways how the CV's and associated nodes can be located in the rectangular flow domain (Patankar, 1980). In this study we have chosen the node centred CV's (Fig. 4A), as indicated to be the best by Patankar (1980). The CV's have a unit thickness in the \(y\)-direction, i.e. \(\Delta y = 1\). The width of the columns and thickness of the layers can be variable throughout the flow domain. In this way the CV's can be located such that interfaces between two substrates or interfaces between boundary conditions can be located at the interfaces of CV's. At the boundaries, the nodes are on the boundaries itself - so-called half CV's are used. For each CV Eq. [57] integrated over time is to be solved. In what follows we use the following notation convention (Fig. 4B). The nodes and the CV's are denoted by capital indexes \((i,j)\), while small indices \((i,j)\) refer to an interface between two CV's.
Figure 4  (A) Example of node centred control volumes with "half" control volumes at the boundaries; the hatched area in (A) is enlarged in (B) showing the Control Volume (CV) (shaded area) around node \((I,J)\) including notation conventions.
For example, the interface between \((i,j)\) and \((i+1,j)\) by \((i,j)\), and that between \((i,j)\) and \((i,j-1)\) by \((i,j-1)\). Column width and row thickness are denoted by \(\Delta x_i\) and \(\Delta z_j\) (with capital subscripts), respectively. The distance between nodes in the x and z directions are denoted by \(\Delta x_i\) and \(\Delta z_j\) (with small subscripts), respectively, defined as

\[
\Delta x_i = 0.5 (\Delta x_i + \Delta x_{i+1}),
\]

and

\[
\Delta z_j = 0.5 (\Delta z_j + \Delta z_{j+1}).
\]

The neighbour nodes or corresponding interfaces are referred to by their ‘geographical’ position, i.e. West, East, North or South, for which the subscripts W, E, N and S are used, respectively (Fig. 4B). In the x-direction there are \(N\) columns or nodes, and in the z-direction there are \(M\) layers or nodes. The volume of a CV equals \(CV = \Delta x_i \Delta y \Delta z_j\), where \(\Delta x_i\) and \(\Delta z_j\) can be written as \(\Delta x_i = (x_{i+1} - x_{i-1})\) and \(\Delta z_j = (z_{j+1} - z_{j-1})\), respectively.

### 3.2.3 Integration of the mixed \(\theta-h\) Richards equation

Equation \([57]\), integrated over time, is solved numerically. The five terms on the left-hand side of Eq. \([57]\) will be elaborated separately below. The variables are all evaluated at the new time \(t+\Delta t\), where \(\Delta t\) is the time step (T), except when stated otherwise. Thus a fully implicit or backward Euler scheme is used.

Integrating the first term of Eq. \([57]\) in the x-direction yields

\[
\int_{z_{j-1}}^{z_j} \int_{x_{i-1}}^{x_i} \int_y^{x_i} \frac{\partial}{\partial x} \left( K \frac{\partial h}{\partial x} \right) dt \, dy \, dz = \int_{z_{j-1}}^{z_j} \Delta y \Delta z_j \Delta t. \quad [60]
\]

In evaluating the (horizontal) flux-terms at the CV interfaces on the right-hand side of Eq. \([60]\), one must assume a profile of \(h\) between the nodes, i.e. apply an interpolation. If it is assumed that \(h\) prevails over the CV, then the derivative of \(h\) is not defined at the CV interface (Fig. 5A). To overcome this problem, we assume a piece-wise-linear \(h\) profile, i.e. linear interpolation (Fig. 5B). Then the right-hand side of Eq. \([60]\) can be written as

\[
\left[ K \frac{\partial h}{\partial x} \right]_{x_{i-1}^j}^{x_i} \Delta y \Delta z_j \Delta t = \left( K_{x_{i,j}} \frac{h_{i+1,j} - h_{i,j}}{\Delta x_i} - K_{x_{i,j-1}} \frac{h_{i,j} - h_{i-1,j}}{\Delta x_i} \right) \Delta y \Delta z_j \Delta t, \quad [61]
\]

where \(K_{x_{i,j}}\) and \(K_{x_{i,j-1}}\) are the hydraulic conductivities in the x-direction at the CV interfaces \((i,j)\) and \((i-1,j)\), respectively. The hydraulic conductivities at the interfaces are unknown, only the hydraulic conductivities at the nodes are known. To evaluate \(K\) at the CV-interfaces several averaging methods have been proposed in the literature (e.g. Haverkamp & Vaclim, 1979; Ross & Bristow, 1990; Zaidel & Russo, 1992). In this study we use the weighted geometric averaging method. This simple method performed best in the one-dimensional problems studied by Haverkamp & Vaclim (1979). Since the width of the CV’s may vary, the CV-interface is generally not situated halfway between two nodes. Therefore, a distance weighing factor in the positive x-direction \(w_i\) (1) is defined as

\[
w_{i,j} = \frac{\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}}. \quad [62]
\]

The weighted geometric average for \(K_{x_{i,j}}\) is then given by

\[
K_{x_{i,j}} = K_{ij}^{i+1} \cdot K_{ij}^{i-1, j}. \quad [63]
\]
Figure 5  Profile assumption for pressure head \( h \) between nodes: (A) step-wise profile; (B) piece-wise linear profile. The piece-wise linear profile is used for evaluating the fluxes at the control volume interfaces in the integration scheme.

In the simulation model two alternative weighting methods can be chosen: weighted arithmetic mean or weighted harmonic mean\(^2\).

Likewise, integrating the second term of Eq. [57] but now in the \( z \)-direction yields

\[
\int y \Delta y \int x \Delta x \int z \Delta z \left( \frac{\partial h}{\partial z} \right) dt \, dx \, dy \, dz = \left[ \frac{\partial h}{\partial z} \right]_{z_{i-1}}^{z_i} \Delta x_i \Delta y \Delta t .
\]

The right-hand side of Eq. [60] now is written as (cf. Eq. [61])

\[
\left[ \frac{\partial h}{\partial z} \right]_{z_{i-1}}^{z_i} \Delta x_i \Delta y \Delta t = \left( K_{x,i} \frac{h_{y,j-1} - h_{y,j}}{\Delta z_j} - K_{z,i,j} \frac{h_{y,j-1} - h_{y,j}}{\Delta z_{j-1}} \right) \Delta x_i \Delta y \Delta t ,
\]

where \( K_{x,i} \) and \( K_{z,i,j} \) are the hydraulic conductivities in the \( z \)-direction at the CV interfaces \((i,j)\) and \((i,j-1)\), respectively. Similar as above, the weighted geometric average for \( K_{z,i} \) is given by

\[
K_{z,i,j} = K_{x,i} w_{z_i} K_{z,i,j+1} w_{z_{i+1}} ,
\]

with the distance weighing factor in the positive \( z \)-direction \( w_z \) (1) defined as

\(^2\) Arithmetic: \( K_{z,i} = (1-w_z) K_{z,i} + w_z K_{z,i+1} \), Harmonic: \( K_{z,i} = \left( \frac{1}{w_z (K_{z,i} + w_z K_{z,i+1})} \right)^2 \)
\[ w_{sj} = \frac{\Delta z_{j+1}}{\Delta z_j + \Delta z_{j-1}}. \]  

[67]

Integration of the gravity term, i.e. the third term of Eq. [57], yields

\[
\int_{z_{i-1}}^{z_i} \int_{y_{j-1}}^{y_j} \int_{x_{i-1}}^{x_i} -\frac{\partial K}{\partial z} \, dt \, dx \, dy \, dz = -\left[ K_{x,j} - K_{x,j-1} \right] \Delta x_i \Delta y \Delta z_t. \]  

[68]

Integration of the sink strength term, i.e. the fourth term of Eq. [57], yields

\[
\int_{z_{i-1}}^{z_i} \int_{y_{j-1}}^{y_j} \int_{x_{i-1}}^{x_i} -S_w \, dt \, dx \, dy \, dz = -S_{w,j} \Delta x_i \Delta y \Delta z_t. \]  

[69]

In Eq. [69] the sink strength is assumed to be explicitly known (see Subsection 3.2.5) and constant during the current time step for each control volume.

Integration of the storage term, i.e. the fifth term of Eq. [57], yields

\[
\int_{z_{i-1}}^{z_i} \int_{y_{j-1}}^{y_j} \int_{x_{i-1}}^{x_i} -\frac{\partial \theta}{\partial t} \, dt \, dx \, dy \, dz = -\left[ \theta_{ij} - \theta_{ij}^0 \right] \Delta x_i \Delta y \Delta z_t, \]  

[70]

where \( \theta_{ij} \) denotes the value of the water content at the end of the time step i.e. at time \( t+\Delta t \), and \( \theta^0 \) represents \( \theta \) at time \( t \).

At this time Eq. [53] is numerically approximated, but it is still expressed in two unknowns, i.e. \( \theta \) and \( h \). The \( \theta \) version of the storage term in Eq. [70] will be further elaborated using the procedure of Celia et al. (1990). Due to the non-linear relationships \( K(\theta) \) and \( \theta(h) \), the solution of the numerical equations has to be found by iteration. A modified Picard iteration procedure is applied here. Let the superscript \( k \) denote the values of \( h \) and \( \theta \) at the \( k \)-th level of iteration, then for the next \( (k+1) \) level \( \theta^{k+1} \) is approximated by a truncated Taylor series with respect to \( h \), about \( h_{ij}^{k+1} \)

\[
\theta_{ij}^{k+1} = \theta_{ij}^k + \left. \frac{d \theta}{dh} \right|_{h_{ij}^k} (h_{ij}^{k+1} - h_{ij}^k) \\
= \theta_{ij}^k + C_{ij}^k (h_{ij}^{k+1} - h_{ij}^k),
\]  

[71]

where \( \theta_{ij}^{k+1} \) is the water content corresponding to \( h_{ij}^{k+1} \). Substituting Eq. [71] in Eq. [70] yields

\[
\int_{z_{i-1}}^{z_i} \int_{y_{j-1}}^{y_j} \int_{x_{i-1}}^{x_i} -\frac{\partial \theta}{\partial t} \, dt \, dx \, dy \, dz = -\left( C_{ij}^k (h_{ij}^{k+1} - h_{ij}^k) \right) \Delta x_i \Delta y \Delta z_t. \]  

[72]

The right-hand side of Eq. [72] resembles the numerically approximated left-hand side of the \( h \)-based Richards equation (Eq. [5]), i.e.

\[
C^k (h^{k+1} - h^0).
\]  

[73]

Numerical solutions of the \( h \)-based Richards equation are accompanied with mass balance errors due to the a priori unknown value of \( C \) (e.g. Milly, 1985; Celia et al., 1990; Rathfelder & Abriola, 1994). In particular, problems occur with \( C \) values close to or equal to zero. Thus why is the Celia et al. (1990) approach better than the 'standard' \( h \) approach? This can be easily seen, since the first term on the right-hand side of Eq. [72] vanishes when the iteration process progresses towards the final solution. Thus the magnitude of \( C \) no longer influences the results. Moreover, the second term
on the right-hand side of Eq. [72] takes care of mass conservation in the numerical computation. Of course, the Taylor expansion in Eq. [71] can also be used in the numerical approximation of the h-based Richards equation, as was done by Rathfelder & Abriola (1994), in which case the same approximated equation is obtained as in the mixed \( \theta-h \) approach.

Taking together the results of Eqs. [60]+[61], [64]+[65], [68], [69] and [72], the numerically approximated form of Eq. [53] after rearrangement of terms is

\[
A_i h_{i,j}^{k+1} = A_w h_{i-1,j}^{k+1} + A_e h_{i+1,j}^{k+1} + A_n h_{i,j-1}^{k+1} + A_s h_{i,j+1}^{k+1} + b,
\]

with

\[
A_{W(\text{est})} = \frac{K_{x,i-1}^k \Delta y \Delta z_j}{\Delta x_{i-1}}, \quad A_{E(\text{est})} = \frac{K_{x,i+1}^k \Delta y \Delta z_j}{\Delta x_{i+1}},
\]

\[
A_{N(\text{orth})} = \frac{K_{x,i}^k \Delta x_i \Delta y}{\Delta z_{j-1}}, \quad A_{S(\text{orth})} = \frac{K_{x,i}^k \Delta x_i \Delta y}{\Delta z_{j+1}},
\]

and

\[
b = A_C h_{i,j}^{k} \left[ \rho_{i,j}^{0} - \rho_{i,j}^{2} \right] \Delta x_i \Delta y \Delta z_j - \left[ K_{x,i}^k - K_{x,i}^{k-1} \right] \Delta x_i \Delta y - S_{w,i,j} \Delta x_i \Delta y \Delta z_j,
\]

where

\[
A_C = \frac{C_{i,j}^k \Delta x_i \Delta y \Delta z_j}{\Delta t}.
\]

Finally, \( A \) is defined as

\[
A = A_E + A_W + A_N + A_S + A_C.
\]

The coefficients \( A_w, A_{ew}, A_{en}, \) and \( A_s \) (\( L^2 T^{-1} \)) refer to the hydraulic conductivity at the interfaces between the CV under consideration and its four respective neighbours and CV geometry, and, hence, are always positive. Coefficient \( A_c \) refers to the differential moisture capacity, CV geometry and time step (\( L^2 T^{-1} \)), and \( b \) contains known quantities (\( L^2 T^{-1} \)). For each node the coefficients \( A, A_c, A_e, A_w, A_n, A_s, \) and \( b \) have to be computed. But, when a face is common to two adjacent CV's, the flux across it must be represented by the same expression in the numerical equations for both CV's. This means that \( A_w \) and \( A_e \) are related as

\[
A_{W,i,j} = A_{E,j-1,i},
\]

and \( A_e \) and \( A_n \) are related as

\[
A_{N,i,j} = A_{S,i,j-1}.
\]

At the beginning of the first iteration level, when \( k = 0 \), the first guess is set equal to the linearly extrapolated values according to the time change during the last time step.

### 3.2.4 Handling of boundary conditions for water movement

For the nodes lying on the boundaries, the boundary conditions must be taken into account when integrating Richards equation. For simplicity reasons the superscript notation \( k+1 \) is left out of notation.
Neumann boundary condition

Neumann conditions, i.e. prescribed flux boundary conditions, can be handled very simply, since they come in naturally during the numerical approximation procedure.

At the top boundary a given flux density (LT⁻³) can be represented by the second main term at the RHS (right hand side) of Eq. [65], plus the second main term at the RHS of Eq. [68]:

\[ q_{top} = - \frac{A_{N,ij} h_{ij} - A_{N,ij} h_{ij-1}}{\Delta x_i \Delta y} + K_{z,ij-1}. \]  

[81]

Multiplying \( q_{top} \) by \( \Delta x_i \Delta y \) one obtains the known volume flux (L²T⁻³) which can be assigned to the variable \( b \) of Eq. [76]. The parameter \( A_{N,ij} \) must be set to zero. Thus, the Neumann conditions at the top boundary \( (j = 1) \) can be represented by Eqs. [74], [75], [77] and [78], with

\[ A_{N,ij} = 0, \]  

[82]

and with \( b \) given by

\[ b = A_c h_i^k \left[ \theta_i^k - \theta_i^0 \right] \Delta x_i \Delta y \Delta z_j \Delta t - K_{z,ij} \Delta x_i \Delta y - S_{w,ij} \Delta x_i \Delta y \Delta z_j + q_{top} \Delta x_i \Delta y. \]  

[83]

At the bottom boundary a given flux density (L⁻¹T⁻¹) can be represented by the first main term at the RHS of Eq. [65], plus the first main term at the RHS of Eq. [68]:

\[ q_{bottom} = - \frac{A_{S,ij} h_{ij+1} - A_{S,ij} h_{ij}}{\Delta x_i \Delta y} + K_{z,ij}. \]  

[84]

Multiplying \( q_{bottom} \) by \( \Delta x_i \Delta y \) one obtains the known volume flux (L²T⁻³) which can be assigned to the variable \( b \) of Eq. [76]. The parameter \( A_{S,ij} \) must be set to zero. Thus, the Neumann conditions at the bottom boundary \( (j = M) \) can be represented by Eqs. [74], [75], [77] and [78], with

\[ A_{S,ij} = 0, \]  

[85]

and with \( b \) given by

\[ b = A_c h_i^k \left[ \theta_i^k - \theta_i^0 \right] \Delta x_i \Delta y \Delta z_j \Delta t - K_{z,ij} \Delta x_i \Delta y - S_{w,ij} \Delta x_i \Delta y \Delta z_j + q_{bottom} \Delta x_i \Delta y. \]  

[86]

At the left boundary a given flux density (L⁻¹T⁻¹) can be represented by the second main term at the RHS of Eq. [61]:

\[ q_{left} = - \frac{A_{W,ij} h_{ij} - A_{W,ij} h_{ij-1}}{\Delta z_i \Delta y}. \]  

[87]

Multiplying \( q_{left} \) by \( \Delta z_i \Delta y \) one obtains the known volume flux (L²T⁻³) which can be assigned to the variable \( b \) of Eq. [76]. The parameter \( A_{W,ij} \) must be set to zero. Thus, the Neumann conditions at the left boundary \( (i = 1) \) can be represented by Eqs. [74], [75], [77] and [78], with

\[ A_{W,ij} = 0, \]  

[88]

and with \( b \) given by
\[ b = A_c h_{ij}^k \left[ \left( \theta_{ij}^k - \theta_{ij}^0 \right) \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} - \left[ K_{z,ij}^k - K_{z,ij-1}^k \right] \Delta x_i \Delta y - S_{w,ij} \Delta x_i \Delta y \Delta z_j \right] + q_{\text{left}} \Delta z_j \Delta y. \] \[ \] \[ [89] \]

At the right boundary a given flux density \( \text{LT}^{-1} \) can be represented by the first main term at the RHS of Eq. [61]:

\[ q_{\text{right}} = -\frac{A_{E,ij} h_{i+1,j} - A_{E,ij} h_{ij}}{\Delta z_j \Delta y}. \] \[ \] \[ [90] \]

Multiplying \( q_{\text{right}} \) by \( \Delta z_j \Delta y \) one obtains the known volume flux \( \text{LT}^{-1} \) which can be assigned to the variable \( b \) of Eq. [76]. The parameter \( A_{E,ij} \) must be set to zero. Thus, the Neumann conditions at the right boundary \( (l = N) \) can be represented by Eqs. [74], [75], [77] and [78], with

\[ A_{E,ij} = 0, \] \[ \] \[ [91] \]

and with \( b \) given by

\[ b = A_c h_{ij}^k \left[ \left( \theta_{ij}^k - \theta_{ij}^0 \right) \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} - \left[ K_{z,ij}^k - K_{z,ij-1}^k \right] \Delta x_i \Delta y - S_{w,ij} \Delta x_i \Delta y \Delta z_j \right] + q_{\text{right}} \Delta z_j \Delta y. \] \[ \] \[ [92] \]

Note that \( q_{\text{top}}, q_{\text{bottom}}, q_{\text{left}} \) and \( q_{\text{right}} \) are user-supplied known flux densities, which are used in Eqs. [83], [86], [89] and [92], respectively; they are not computed according to Eqs. [81], [84], [87] and [90]. Positive flux densities, thus water movement in the positive \( x \) or \( z \) direction, at the left and top boundaries are added to \( b \) (water entry) as in Eqs. [83] and [89], while at the right and bottom boundaries a positive flux density means outflow of water and thus their magnitudes are subtracted from \( b \) as in Eqs. [86] and [92]. The procedure becomes clear when one considers one CV and the intermediate steps in obtaining Eq. [74] are fully written down. In that case, one obtains the following equation (disregarding the sink strength term)

\[ \left( A_{E,ij} h_{i+1,j} - A_{E,ij} h_{ij} \right) - \left( A_{W,ij} h_{ij} - A_{W,ij} h_{i-1,j} \right) + \left( A_{S,ij} h_{ij+1} - A_{S,ij} h_{ij-1} \right) - \left( A_{N,ij} h_{ij} - A_{N,ij} h_{ij-1} \right) + \left( K_{z,ij}^k - K_{z,ij-1}^k \right) \Delta x_i \Delta y \Delta z_j \Delta t = 0. \] \[ \] \[ [93] \]

With the definitions of \( q_{\text{top}}, q_{\text{bottom}}, q_{\text{left}}, q_{\text{right}} \) in Eqs. [81], [84], [87] and [90], Eq. [93] can be written as

\[ -q_{\text{right}} \Delta z_j \Delta y + q_{\text{left}} \Delta z_j \Delta y - q_{\text{bottom}} \Delta x_i \Delta y + q_{\text{top}} \Delta x_i \Delta y + A_{C,ij} \left( h_{ij} - h_{ij}^k \right) \left( \theta_{ij}^k - \theta_{ij}^0 \right) \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} = 0. \] \[ \] \[ [94] \]

In fact, the mass balance equation states the difference between what comes in and what goes out.

Flux boundary conditions at the bottom defined by Eq. [14] (unit gradient) or by Eqs. [15]-[16] (resistance drain) are computed according to the corresponding equations and then these fluxes \( q_{\text{bottom}} \) are used in the numerical computations.
**Dirichlet boundary condition**

The Dirichlet or pressure head boundary condition could be handled by setting \( A_r = A_w = A_z = A_u = 0 \), \( A = 1 \) and \( b = h_r \), with \( h_r \) being the prescribed pressure head (L). However, for one of the solution methods used in the model, i.e. the ICCG solution procedure, this would result in a non-symmetric coefficient matrix\(^3\), and, thus, cannot be used. Therefore, a numerical trick is used as an alternative (Wang & Anderson, 1982; Larabi & De Smedt, 1994). Eqs. [74], [75] and [77] are used, and \( b \) is given by

\[
b = h_r L.
\]  
[95]

and \( A \) is given by

\[
A = L.
\]  
[96]

In Eqs. [95] and [96] the variable \( L \) is some large number, e.g. \( L = 10^{35} \). In that way the other terms in Eq. [74] are insignificant during the computations, i.e. Eq. [74] is nearly equal to

\[
A h^{k+1}_{i,j} = b,
\]  
[97]

so that, with Eqs. [95] and [96], the newly calculated pressure head is forced to the desired value:

\[
h^{k+1}_{i,j} = h_T.
\]  
[98]

One should be aware of possible overflow problems as a result of this; however, they did not occur in our computations.

**Boundary conditions and nodes at a corner of the flow domain**

Nodes situated in the control volumes at the corners of the flow domain are subject to two boundary conditions. For example, the upper left node is subject to the condition at the surface and at the left boundary. Theoretically, four different situations may exist, since either boundary can be of Dirichlet or Neumann type. In the simulation model care is taken that all possible situations can be dealt with. When both are of Neumann type, the two known fluxes are added to \( b \), analogously as described above. When one is of Neumann type and the other of Dirichlet type, the pressure head of the node is forced to the desired value, and the known flux is added to \( b \). When both are of Dirichlet type, both prescribed pressure heads should be the same, otherwise two conditions exist for one node, which cannot be treated by the current model.

**Seepage faces**

During the iterations it is checked which of the conditions specified by Eqs. [12] and [13] prevails at (part of) the seepage face. The Dirichlet and Neumann parts of the seepage face are then treated in the same way as other boundary conditions, as described above.

**Specified conditions for internal nodes**

It is possible that at certain internal nodes specified conditions exist. A prescribed pressure head (Dirichlet condition) is treated similarly as described above for boundary nodes. A prescribed flux density is treated as a known source or sink. Equations [74]-[78] are used, with the source or sink term, \( q_{\text{intern}} \), added to the \( b \) parameter in Eq. [76]:

\[
b = A_c h_{i,j}^{k} - \left[ \vartheta_{i,j}^{k} - \vartheta_{i,j}^{k+1} \right] \Delta x_i \Delta y_i \Delta z_j - \left[ K_{x,i,j}^{k} - K_{x,i,j-1}^{k} \right] \Delta x_i \Delta y_i \Delta z_j - S_{w,i,j} \Delta x_i \Delta y_i \Delta z_j + q_{\text{intern}} \Delta x_i \Delta z_j.
\]  
[99]

**Computation of flux densities**

Water flux densities across the CV interfaces are needed for the solute transport computations. So,
when the new \( h \) distribution is known, the water flux densities based on Darcy’s law (Eq. [2]) can be computed. For all interfaces other than the boundaries the flux density in the \( x \)-direction, \( F_x \) (L\( \cdot \)L\( \cdot \)T\(^{-1} \)), is given by (gravity does not play a role)

\[
q_{x,ij} = -K_{x,ij} \frac{h_{i+1,j} - h_{i,j}}{\Delta x_i}.
\]

For all interfaces other than the boundaries the flux density in the \( z \)-direction, \( F_z \) (L\( \cdot \)L\( \cdot \)T\(^{-1} \)), is given by (including gravity)

\[
q_{z,ij} = -K_{z,ij} \frac{h_{i,j+1} - h_{i,j}}{\Delta z_j} + K_{z,ij}.
\]

At the boundaries the boundary conditions are considered. For a Neumann type condition it is obvious that the corresponding flux density equals the prescribed flux density. When a Dirichlet condition exists, the flux density across the boundary must balance the net flux density across the other interfaces and the sink term. Thus, at the top boundary we have

\[
q_{z,ij} = q_{z,ij} + (q_{k,ij} - q_{k,j-1,j}) \frac{\Delta z_j}{\Delta x_j} \frac{S_{w,ij}}{\Delta x_j}.
\]

At the bottom boundary we have

\[
q_{z,ij} = q_{z,ij-1} - (q_{k,ij} - q_{k,j-1,j}) \frac{\Delta x_j}{\Delta z_j} \frac{S_{w,ij}}{\Delta z_j}.
\]

At the left boundary we have

\[
q_{x,i-1,j} = q_{x,i,j} + (q_{z,i,j} - q_{z,i,j-1}) \frac{\Delta x_j}{\Delta z_j} \frac{S_{w,ij}}{\Delta z_j}.
\]

At the right boundary we have

\[
q_{x,i,j} = q_{x,i-1,j} - (q_{z,i,j} - q_{z,i,j-1}) \frac{\Delta x_j}{\Delta z_j} \frac{S_{w,ij}}{\Delta z_j}.
\]

The same computations hold for boundary nodes subject to two boundary conditions (i.e. corner nodes), except when both sides of the CV at a corner are of Neuman type. In that case, the net amount of water inflow is equally divided over the two sides.

### 3.2.5 Root water uptake

The root water uptake model as described in Section 2.3 considers a single layer of porous medium with uniform root length density. For a root system distributed over several control volumes, it is assumed that within each control volume the roots are regularly distributed, so that for each control volume the model described in Section 2.3 can be applied. The sink strength for each control volume is then given by (combining Eqs. [20] and [22])
\[ \Delta z_i S_{w,i,j} = \Delta z_i L_{w,i,j} K_1 (h_{\text{r},i,j} - h_i + \sigma_i (h_{o,i,s} - h_{o,i})) = \]
\[ = \pi \Delta z_i L_{w,i,j} \frac{P_{ij}^2 - 1}{G_o (\rho_{ij})} (\phi_{ij} - \phi_{r,i,j}). \]

Note that \( S_{w,i,j} = q_i / \Delta z_i = q_j / \Delta z_j \). The sum of all sink strengths then equals the actual transpiration rate \( T \) (cf. Eq. [18])
\[ T = \sum_{i=1}^{N} \sum_{j=1}^{M} \Delta z_i S_{w,i,j}. \]

\( T \) is a function of the root pressure head \( h \), and the potential transpiration rate \( T_p \) as described by Eqs. [25] and [26]. \( K_r, h_r, R_o, \sigma \) and \( h_{o,r} \), are assumed to be constant for the whole root system, and \( h \) and \( h_r \) (from Eq. [44], using EC data of previous time step) of the bulk soil in the CV is assumed to be known. This results in a set of \((N \times M + 1)\) equations with \((N \times M + 1)\) unknowns: \( N \times M \) values of \( h_r \) and \( h_r \). However, due to the non-linear relationship between \( h \) and \( \phi \) on the one hand and \( h \) and \( T \) on the other hand, the solution has to be found iteratively. The procedure consists of two steps. In the first step two estimates for \( h_r \) are obtained for which the sum of all root water uptake is less than and more than \( T \), respectively. Secondly, the true value for \( h_r \) is computed in the range bounded by these two estimates. \( \phi \) is evaluated according to the procedure described in Appendix 1. Although \( \phi \) is defined by Eq. [23] we approximate it from \( h \) in the bulk substrate in the CV.

In short the procedure is as follows. In the first step one starts with \( T = T_p \). The first estimate of \( h_r \) is obtained according to Eq. [28] as
\[ h_r = \frac{K_1 \sum_{i=1}^{N} \sum_{j=1}^{M} L_{w,i,j} \Delta x_i \Delta z_j (h_{i,j} - \sigma_i h_{o,i,j}) + T_p \sum_{i=1}^{N} \Delta x_i}{K_1 \sum_{i=1}^{N} \sum_{j=1}^{M} L_{w,i,j} \Delta x_i \Delta z_j} + \sigma h_{o,r}. \]

Then, equation [106] is solved for \( h_r \) using e.g. the method of false position (Press et al., 1986). The sum of all computed root water uptakes is compared with \( T \), cf. Eq. [107]. If total uptake is smaller (larger) than \( T \), then current \( h_r \) is the lower (upper) limit. The upper (lower) limit is found by - repeatedly - increasing the current estimate of \( h \), with a certain factor, e.g. 5; \( T \) is adapted as well (according to Eq. [26]). In the second step the true value of \( h_r \) is obtained using the method of false position within the lower and upper limit range obtained in the first step. Convergence is reached when
\[ \sum_{i=1}^{N} \sum_{j=1}^{M} \Delta z_i S_{w,i,j} - T \leq \epsilon_i, \]
where \( \epsilon_i \) is some small number, e.g. \( \epsilon_i = 0.01 \). The corresponding sink strengths can then be used in Eq. [76]. Thus root water uptake is considered explicitly.

In the simulation model there is an option to consider root water uptake to occur as water uptake from a CV proportional to root length present in a CV. It is assumed that the roots form the limiting factor in water uptake, that water movement from the bulk soil to the roots can always be satisfied, that the soil is wet, and that osmotic effects do not play a role. Under these circumstances \( h \approx h_{r}, \) \( h_r = h \) and \( \sigma = 0 \). Expressing uptake of water on a volume basis it follows from Eq. [20] that
\[ S_{w,i,j} \Delta x_i \Delta y \Delta z_j = - \Delta x_i \Delta y \Delta z_j L_{w,i,j} K_1 h_r. \]

The sum of all water taken up is equal to the transpiration rate times the soil surface (combining Eqs. [28] and [107]):
\[
\Delta y \sum_{i}^{N} \sum_{j}^{M} S_{w,i,j} \Delta x_{i} \Delta z_{j} = - K_{i} h_{i} \Delta y \sum_{i}^{N} \sum_{j}^{M} \Delta x_{i} \Delta z_{j} L_{v,i,j} = \Delta y \sum_{i}^{N} \Delta x_{i} .
\]  \[111\]

From the second part of Eq. [111] the following expression for \( h_{i} \) can be obtained (cf. Eq. [28])

\[
h_{i} = - \frac{\Delta y \sum_{i}^{N} \Delta x_{i}}{K_{i} \Delta y \sum_{i}^{N} \sum_{j}^{M} \Delta x_{i} \Delta z_{j} L_{v,i,j}} .
\]  \[112\]

Substituting Eq. [112] in [110] yields \( S_{w,i,j} \) representing water uptake from a CV proportional to root length present in a CV:

\[
S_{w,i,j} = \frac{L_{v,i,j} \sum_{i}^{N} \Delta x_{i}}{\sum_{i}^{N} \sum_{j}^{M} L_{v,i,j} \Delta x_{i} \Delta z_{j}} .
\]  \[113\]

### 3.3 Solution of the matrix equation for water movement

For each node Eq. [74] holds, and the total problem can be presented in matrix notation as

\[
A \ h = b ,
\]  \[114\]

where \( A \) is a coefficient matrix of \((N \times M)\) by \((N \times M)\), and the vectors \( h \) and \( b \) of length \((N \times M)\) contain the unknown values of \( h \) and the known values of \( b \), respectively. For the CV method the coefficient matrix \( A \) contains the coefficients \( A_{e}, A_{v}, A_{w}, A_{r}, \) and \( A_{n} \) stored in 5 bands (Fig. 6). Matrix \( A \) is symmetric due to Eqs. [79] and [80], sparse since most elements are zero, positive definite, and all elements outside the main diagonal are less than or equal to zero, \( A \) is non-singular and \( A^{-1} > 0 \), i.e. \( A \) is a so-called M-matrix (Meijerink & Van Der Vorst, 1977; Larabi & De Smedt, 1994). Due to the simple sparsity pattern, storage is easy.

The solution of Eq. [114] is

\[
h = A^{-1} b .
\]  \[115\]

However, it is often time-consuming to find the inverse matrix of \( A \). A direct method of solving the problem is by the Gauss-Seidel elimination method. This method is known to be time-consuming, especially for a large number of CV’s. In the literature some alternative methods have been proposed. A very simple and fast method is the Alternating Direction Implicit (ADI) method, first proposed for multi-dimensional parabolic and elliptic (linear) partial differential equations by Peaceman & Rachford (1955). The ADI method functions well for unsaturated problems (Heinen & De Willigen, 1992). But when regions partly saturated and partly unsaturated were considered, the ADI method failed. An alternative method is the Incomplete Cholesky Conjugate Gradient (ICCG) method (Meijerink & Van Der Vorst, 1977; Kershaw, 1978; Kuiper, 1981; Golub & Van Loan, 1989), which recently is used frequently in partly saturated regions (e.g. Kuiper, 1981; Kirkland et al., 1992; Larabi & De Smedt, 1994). These methods were originally developed for linear problems, but they can be used in the iteration step since within the iteration the problem is linear. The ADI method is described in Subsection 3.3.1 and the ICCG method in Subsection 3.3.2. In what follows reference is made to internal nodes. The same reasoning holds, however, for boundary nodes.
3.3.1 Alternating Direction Implicit (ADI) method

The ADI method for a two-dimensional case consists of two steps. In the first step the equations are written implicitly in one direction (e.g. x) and explicitly in the other direction (e.g. z). In step two the opposite procedure is followed: explicitly in the first direction and implicitly in the second direction. For each step the resulting matrix equation is solved, with the solution of the first step used in the second step. Solution of the equations obtained in the second step then completes one iteration step.

**Step 1**
Assume that all values are known at iteration level $k$, writing Eq. [74] implicitly in the $x$-direction yields

$$A h_{i,j}^{k+1/2} = A_w h_{i-1,j}^{k+1/2} + A_e h_{i+1,j}^{k+1/2} + b.$$ \[116\]

The coefficients $A_e$, $A_w$, $A_u$, $A_N$, and $A_c$ are the same as given in Eqs. [75] and [77], and $A$ is

$$A = A_e + A_w + A_c,$$ \[117\]

and $b$ is...
\[ b = A_c h_{i,j}^k - (\partial_{x_{i,j}^k} - \partial_{x_{j,j}^k}) \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} - A_i [h_{i,j}^k - h_{i,j+1}^k] - A_N [h_{i,j}^k - h_{i,j-1}^k] + \]
\[ - [K_{i,j}^k - K_{i+1,j}^k] \Delta x_i \Delta y - S_{w,i,j} \Delta x_i \Delta y \Delta z_j. \]

[118]

This procedure thus yields a system of \( M \) equations for each of the \( N \) rows in the \( z \)-direction. The equations can be presented in a form analogous to Eq. [114], but now \( A \) has only the three main bands filled with non-zero values, i.e. the main diagonal plus the bands directly above and directly below the main diagonal, and vector \( b \) contains also the explicit terms. This set of equations can be solved efficiently and quickly by a special form of the Gauss-Seidel elimination method known as the Thomas algorithm (e.g. Press et al., 1986).

**Step 2**

So the values of \( h_{i,j}^{k+1/2} \) are obtained and from these \( K_{i,j}^{k+1/2} \) and \( \partial_{x_{i,j}^{k+1/2}} \). After calculation of the average values of the conductivity at the faces of the CV's the equations are written implicitly in the \( z \)-direction

\[ A h_{i,j}^{k+1} = A_N h_{i,j+1}^{k+1} + A_i h_{i,j+1}^{k+1} + b. \]

[119]

The coefficients \( A_i, A_w, A_D, A_N \), and \( A_c \) are as given in Eqs. [75] and [77] with all hydraulic properties evaluated at iteration level \( k+1/2 \), whereas \( A \) is

\[ A = A_N + A_i + A_c, \]

[120]

and \( b \) is

\[ b = A_c h_{i,j}^{k+1/2} - (\partial_{x_{i,j}^{k+1/2}} - \partial_{x_{j,j}^{k+1/2}}) \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} - A_i [h_{i,j}^{k+1/2} - h_{i+1,j}^{k+1/2}] - A_W [h_{i,j}^{k+1/2} - h_{i,j-1}^{k+1/2}] - [K_{k,j}^{k+1/2} - K_{k+1,j}^{k+1/2}] \Delta x_i \Delta y - S_{w,i,j} \Delta x_i \Delta y \Delta z_j, \]

[121]

Solution of the \( N \) equations at the \( M \) columns in the \( x \)-direction yields the values of \( h_{i,j}^{k+1} \) at the iteration level \( k+1 \).

The ADI method can be used either for parabolic and for elliptic partial differential equations (Peaceman & Rachford, 1955; Rosenberg, 1969). However, according to the literature, for parabolic problems the complete time step should be used in both ADI steps, while for elliptic problems half the time step should be used in each of the two ADI steps. When variably saturated conditions exist in the flow domain, part of the problem is parabolic (unsaturated zone) and the rest is elliptic (saturated zone). In that case it is known what time step to be used. Peaceman & Rachford (1955) and Douglas et al. (1959) used an iteration parameter to speed up convergence for elliptic problems. This concept was successfully used by Rubin (1968) in partly saturated porous media, but our attempt failed. Another attempt to solve the mixed parabolic-elliptic problem is to force the Richards equation in the saturated part of the porous medium to stay parabolic by introducing a compressibility coefficient as was done by e.g. Russo et al. (1994).

In this study the ADI method was successfully implemented as follows. In Eq. [118] it can be seen that the vertical flux densities across the horizontal interfaces are treated explicitly. In these expressions the unknown pressure head at the central node, \( h_{i,j} \) is also present. In the alternative ADI solution procedure, which is used when partially saturated condition exist, the terms containing \( h_{i,j} \) are moved from the knowns vector \( b \) in Eq. [118] and incorporated to the left hand side of Eq. [116], so that the parameter \( A \) is no longer given by Eq. [117] but by Eq. [78]. Analogously, the second ADI step is handled. Thus, Eqs. [116]-[121] are replaced by the following set of equations.

**Step 1**

Implicitly in the \( x \)-direction
\begin{equation}
A \ h_{ij}^{k+\frac{1}{2}} = A_w \ h_{i-1,j}^{k+\frac{1}{2}} + A_e \ h_{i+1,j}^{k+\frac{1}{2}} + b.
\end{equation}  
[122]

The coefficients \( A_e, A_w, A_s, A_h \) and \( A \) are the same as given in Eqs. [75] and [77], and \( A \) is

\begin{equation}
A = A_N + A_s + A_e + A_w + A_C,
\end{equation}  
[123]

and \( b \) is

\begin{equation}
b = A_e h_{ij}^k - \left[ \partial_i^2 - \partial_j^2 \right] \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} + A_s h_{i+1,j}^k + A_N h_{ij-1}^k +
\end{equation}  
[124]

\begin{equation}
- \left[ K_{z_{ij}}^k - K_{z_{ij-1}}^k \right] \Delta x_i \Delta y - S_{w_{ij}} \Delta x_i \Delta y \Delta z_j.
\end{equation}

**Step 2**

Implicitly in the \( z \)-direction

\begin{equation}
A \ h_{ij}^{k+1} = A_N h_{i-1,j}^{k+1} + A_s h_{i+1,j}^{k+1} + b.
\end{equation}  
[125]

The coefficients \( A_e, A_w, A_s, A_h \) and \( A \) are as given in Eqs. [75] and [77] with all hydraulic properties evaluated at iteration level \( k+1/2 \), whereas \( A \) is

\begin{equation}
A = A_N + A_s + A_e + A_w + A_C,
\end{equation}  
[126]

and \( b \) is

\begin{equation}
b = A_e h_{ij}^{k+\frac{1}{2}} - \left[ \partial_i^{k+\frac{1}{2}} - \partial_j^{k+\frac{1}{2}} \right] \frac{\Delta x_i \Delta y \Delta z_j}{\Delta t} - A_s h_{i+1,j}^{k+\frac{1}{2}} + A_N h_{ij-1}^{k+\frac{1}{2}} +
\end{equation}  
[127]

\begin{equation}
- \left[ K_{z_{ij}}^{k+\frac{1}{2}} - K_{z_{ij-1}}^{k+\frac{1}{2}} \right] \Delta x_i \Delta y - S_{w_{ij}} \Delta x_i \Delta y \Delta z_j.
\end{equation}

With this version of ADI larger mass balance errors were obtained (see Chapter 6).

### 3.3.2 Incomplete Cholesky Conjugate Gradient (ICCG) method

The M-type coefficient matrix \( A \) (see Section 3.3) is generated by numerical approximation of the elliptic equation, as is the Laplace equation in the saturated zone, and the parabolic differential equation, as is the Richards equation for the unsaturated zone. In that case, a promising method to solve Eq. [114] is the ICCG method (Meijerink & Van Der Vorst, 1977). The ICCG method works as follows.

Matrix \( A \) in Eq. [114] is replaced by a preconditioning matrix \( C \), so that the system can be solved easier. Here matrix \( C \) is defined as the Cholesky decomposition matrix

\begin{equation}
C = LL^T,
\end{equation}  
[128]

where \( L \) is the Cholesky lower triangular matrix, and \( L^T \) is its transpose matrix and thus upper triangular. The elements of \( L \) are computed as

\begin{equation}
\text{for } A_{yi} \neq 0 \quad \frac{1}{L_{yi}} = \frac{1}{L_{yi}} \left( A_{yi} - \sum_{x=1}^{y-1} L_{ix}L_{yx} \right),
\end{equation}  
[129]

\begin{equation}
\text{for } A_{yi} = 0 \quad L_{yi} = 0,
\end{equation}

\( \gamma = t_1(t+1), (t+2), \ldots, (N \cdot M) \).
The first and second indices refer to the column and row numbers of the matrix, respectively. For the special case of the five-banded matrix $A$ in this study, the product of $L_x L_y$ in the first part of Eq. [129] is always zero, and thus the summation term disappears. The procedure is called incomplete Cholesky decomposition, since the same sparsity pattern as for $A$ is forced on $C$, as is stated in the second part of Eq. [129]. Thus storage of the elements of $C$ can be done in the same way as for $A$. The discarded entries are generally small, and the incomplete construction is at least as stable as the complete construction (Meijerink & Van Der Vorst, 1977; Gustafsson, 1984). The benefit of the ICCG method is that the solution of the matrix equation

$$Ch = b,$$  \[130\]

is obtained in two simple steps: first, by forward substitution of

$$Ly = b,$$  \[131\]

followed by backward substitution of

$$L^T h = y,$$  \[132\]

to obtain the solution $h$, where vector $y$ is an intermediate dummy vector.

Since $C$ is not equal to $A$, the solution cannot be found directly, and iterations are needed. Here we use the conjugate gradient iterative solution (Hestenes & Stiefel, 1952; Meijerink & Van Der Vorst, 1977; Kershaw, 1978; Golub & Van Loan, 1989; Larabi & De Smedt, 1994). The conjugate gradient method is simpler to code and requires less storage space than the standard Gaussian elimination method.

For any arbitrary initial estimate $h^0$, the initial values for the residual vector $r$ (being the difference between the current estimated solution and the exact solution) and direction vector $p$ (being the vector pointing from the current estimated solution to the exact solution) are computed from (Kershaw, 1978)

$$r^0 = b - A h^0,$$  \[133\]

$$p^0 = (L L^T)^{-1} r^0.$$

The solution is computed according to (Kershaw, 1978)

$$a_1^t = \frac{\{r^t, (L L^T)^{-1} r^t\}}{\{p^t, A p^t\}},$$

$$h^{t+1} = h^t + a_1^t p^t,$$

$$r^{t+1} = r^t - a_1^t A p^t,$$  \[134\]

$$a_2^t = \frac{\{r^{t+1}, (L L^T)^{-1} r^{t+1}\}}{\{r^t, (L L^T)^{-1} r^t\}},$$

$$p^{t+1} = (L L^T)^{-1} r^{t+1} + a_2^t p^t,$$

$$\lambda = 0, 1, 2, \ldots$$

The scalars $a_1$ and $a_2$ are iteration parameters which are used to refine the vectors $r$ and $p$, respectively, the parameter $\lambda$ is the local iteration counter, and the notation $\{,\}$ represents the inner product of two vectors, and $r$ is a scalar value. Normally, after $\lambda = MxN$ iterations the solution is obtained. However, due to rounding-off errors and since $LL^T$ is only approximately equal to $A$, this may not be the case. It is obvious that the more $C$ resembles $A$ the less iterations are needed. Due to the simple sparsity pattern of $A$ and $C$, the computations can be carried out easily. Convergence is achieved as soon as for all nodes the relative difference $d_i$ between all corresponding elements
of $h^{4+1}$ and $h^{4}$ is less than a small value $\epsilon_i$, e.g. $\epsilon_i = 10^{-6}$, with $d_i$ defined as

$$d_i = \frac{|h^{4+1} - h^4|}{|h^{4+1}| + 100.0}.$$  \[135\]

For absolute large values of $h$ Eq. [135] gives approximate relative changes. In case $h$ becomes close to zero, Eq. [135] gives approximate absolute changes divided by 100. For near zero values of $h$, relative changes would be difficult to compute, and convergence is not guaranteed; therefore, the factor 100 was introduced in Eq. [135].

The incomplete Cholesky conjugate gradient method was developed for linear systems. For nonlinear systems this method can be used in the main iteration loop, then for each iteration the system is assumed to be linear.

### 3.3.3 Convergence criterion

To determine if convergence is achieved in the main iteration process, the maximum relative change in $K$ or $h$ is computed according to

$$d = \max(d_1, d_2),$$  \[136\]

with

$$d_1 = \frac{|h_{ij}^{k+1} - h_{ij}^k|}{|h_{ij}^{k+1}| + 100.0},$$  \[137\]

and

$$d_2 = \frac{|K_{ij}^{k+1} - K_{ij}^k|}{K_{ij}^{k+1} + 100.0},$$  \[138\]

where in Eq. [136] the operator $\max$ yields the maximum value of its arguments. Iterations are halted when for all nodes $d$ is smaller than a small number $\epsilon$, e.g. $\epsilon = 10^{-4}$. Equations [137] and [138] are of the same form as Eq. [135] (see also discussion below Eq. [135]).

For not too wet conditions, the largest changes will be in $K$ rather than in $h$. Heinen & De Willigen (1992) determined the pressure head above which the largest changes occur in $h$ for sand, clay, peat and loamy sand soils; they obtained values of $h$ in the range -3 cm to -22 cm.

### 3.4 Explicit solution for nutrient transport

Opposite to the water movement described above, nutrient transport is considered explicitly. However, use is made of the results of the water movement computations. The nutrient flux density is described in Subsection 3.4.1, and the handling of boundary conditions in Subsection 3.4.2. Nutrient uptake by the root system is described in Subsection 3.4.3.

#### 3.4.1 Nutrient flux density

Solute transport is solved explicitly, i.e. the solute mass flux densities are evaluated at the control volume (CV) interfaces using the water flux densities obtained at $t+\Delta t$ and from that the dispersion-diffusion coefficients at $t+\Delta t$, and the concentrations at time $t$. The solute flux at a CV interface consists of a convective part and two dispersion-diffusion parts, one due to a gradient in $c$ perpendicular to the interface, and one due to a gradient in $c$ parallel to the interface. The three
parts will be computed separately and then summed. Once all solute fluxes are known the change in total amount $Q$ in each CV can be computed and from that the new $c$.

The governing solute transport equation expressed in $Q$, Eq. [29] or [32], is here written in two dimensions as

$$
\frac{\partial Q}{\partial t} = -\frac{\partial q_{xx} c}{\partial x} - \frac{\partial q_{xz} c}{\partial z} + \frac{\partial}{\partial x} \left( \theta D_{xx} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial z} \left( \theta D_{zz} \frac{\partial c}{\partial z} \right) +
$$

$$
+ \frac{\partial}{\partial x} \left( \theta D_{xz} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial z} \left( \theta D_{zx} \frac{\partial c}{\partial z} \right) - S_s,
$$

[139]

or

$$
\frac{\partial Q}{\partial t} = -\frac{\partial q_{xx}^c}{\partial x} - \frac{\partial q_{xz}^c}{\partial z} - \frac{\partial q_{sx}^d}{\partial x} - \frac{\partial q_{sz}^d}{\partial z} - \frac{\partial q_{dz}^d}{\partial x} - \frac{\partial q_{sz}^d}{\partial z} - S_s,
$$

[140]

where

$$
q_{sx}^c = q_x c,
$$

[141]

$$
q_{sz}^c = q_z c,
$$

and

$$
q_{sx}^d = -\theta D_{sx} \frac{\partial c}{\partial x},
$$

[142]

$$
q_{sz}^d = -\theta D_{sz} \frac{\partial c}{\partial z},
$$

$$
q_{sx}^d = -\theta D_{x} \frac{\partial c}{\partial x},
$$

$$
q_{sz}^d = -\theta D_{z} \frac{\partial c}{\partial z},
$$

Superscripts $d$ and $c$ refer to dispersion-diffusion and convection, respectively. Eq. [140] can be reduced to

$$
\frac{\partial Q}{\partial t} = \frac{\partial q_{sx}}{\partial x} - \frac{\partial q_{sz}}{\partial z} - S_s,
$$

[143]

where

$$
q_{sx} = q_{sx}^c + q_{sx}^d + q_{sz}^d,
$$

[144]

$$
q_{sz} = q_{sz}^c + q_{sz}^d + q_{sz}^d.
$$

The expressions between the brackets of the fifth and sixth terms on the right-hand side of Eq. [139], i.e. $q_{sx}^d$ and $q_{sz}^d$ (Eq. [140]), represent the solute fluxes in the $x$ and $z$ direction caused by gradients of $c$ in the $z$ and $x$ directions, respectively. $S_s$ is assumed to be explicitly known. The new distribution of the solutes follows from Eq. [143]. The total mass $Q_{m} (M)$ of a CV is defined as (Eq. [47])

$$
Q_{m,j} = Q_{i,j} \Delta x_j \Delta y \Delta z_j.
$$

[145]

Using Eq. [145], Eq. [143] is now rewritten as

$$
\frac{\partial Q_{m,j}}{\partial t} = \left( -\frac{\partial q_{sx,j}}{\partial x} - \frac{\partial q_{sz,j}}{\partial z} - S_{s,j} \right) \Delta x_j \Delta y \Delta z_j.
$$

[146]
Equation [146] is numerically solved as
\[
\frac{Q^{t+\Delta t}_{m,l,j} - Q^{t}_{m,l,j}}{\Delta t} = \frac{q^{t+\Delta t}_{sx,l-1,j} - q^{t+\Delta t}_{sx,l,j}}{\Delta x_i} \Delta y \Delta z_j + \frac{q^{t+\Delta t}_{sz,l-1,j} - q^{t+\Delta t}_{sz,l,j}}{\Delta z_j} \Delta x_i \Delta y \Delta z_j + \frac{q^{t+\Delta t}_{sz,l,j} - q^{t+\Delta t}_{sz,l+1,j}}{\Delta z_j} \Delta x_i \Delta y \Delta z_j,
\]
so that
\[
Q^{t+\Delta t}_{m,l,j} = Q^{t}_{m,l,j} + \left( q^{t+\Delta t}_{sx,l-1,j} - q^{t+\Delta t}_{sx,l,j} \right) \Delta y \Delta z_j \Delta t + \left( q^{t+\Delta t}_{sz,l-1,j} - q^{t+\Delta t}_{sz,l,j} \right) \Delta x_i \Delta y \Delta t + \left( q^{t+\Delta t}_{sz,l,j} - q^{t+\Delta t}_{sz,l+1,j} \right) \Delta x_i \Delta y \Delta z_j \Delta t,
\]
The concentration \( c \) in CV \((l,j)\) can be computed from (cf. Eq. [30])
\[
c^{t+\Delta t}_{l,j} = \frac{Q^{t+\Delta t}_{m,l,j}}{\theta^{t+\Delta t}_{l,j} \Delta x_i \Delta y \Delta z_j}.
\]
The total solute flux densities at the CV interfaces appearing in Eq. [148] are evaluated by Eq. [144] plus Eqs. [141] and [142]. The convective and dispersive-diffusive solute flux densities are obtained in the following two sections.

**Convection**
The convective parts of \( q \), Eq. [141], at the CV interfaces are obtained using the method of upstream weighing (e.g. Patankar, 1980):
\[
\text{if } q^{t+\Delta t}_{sx,l,j} \geq 0 \quad q^{c^{t+\Delta t}}_{sx,l,j} = q^{t+\Delta t}_{sx,l,j} c^{t}_{l,j},
\]
\[
\text{if } q^{t+\Delta t}_{sx,l,j} < 0 \quad q^{c^{t+\Delta t}}_{sx,l,j} = q^{t+\Delta t}_{sx,l,j} c^{t}_{l+1,j},
\]
and
\[
\text{if } q^{t+\Delta t}_{sz,l,j} \geq 0 \quad q^{c^{t+\Delta t}}_{sz,l,j} = q^{t+\Delta t}_{sz,l,j} c^{t}_{l,j},
\]
\[
\text{if } q^{t+\Delta t}_{sz,l,j} < 0 \quad q^{c^{t+\Delta t}}_{sz,l,j} = q^{t+\Delta t}_{sz,l,j} c^{t}_{l-1,j}.
\]
Thus, if the Darcy water flux density is from node A to node B, the nutrient flux density is the water flux density times \( c \) at node A. Using the upstream weighing method numerical oscillations are minimized. But still small oscillations and numerical dispersion may exist, especially in explicit schemes. Daus et al. (1985) concluded that, for a one-dimensional problem, stability is achieved when at all positions in the flow domain the Fourier number is smaller than 0.5. The Fourier number \( (Fo) \) is defined as the ratio of the Courant \( (Co) \) and Peclet \( (Pe) \) numbers. The \( Pe, Co \) and \( Fo \) numbers (1) are defined as (e.g. Daus et al., 1985; El-Kadi & Ling, 1993)
\[
P_{e_{l,j}} = \frac{| q^{n}_{l,j} | \Delta S_{l,j} }{ \theta_{l,j} D_{l,j} },
\]
\[
C_{o_{l,j}} = \frac{| q^{n}_{l,j} | \Delta t }{ \theta_{l,j} S_{l,j} },
\]
and

\[ \text{Fo}_{i,j} = \frac{C_{i,j}}{P_{e_{i,j}}} = \frac{D_{i,j} \Delta t}{(\Delta s_{i,j})^2}, \]

where \( \Delta s_{i,j} \) is the characteristic length of control volume \((i,j)\) (L), here chosen to be the minimum of \( \Delta x_i \) and \( \Delta z_j \) of that CV, and \( q_{i,j}^n \) is the magnitude of net flux density into CV \((i,j)\). Simunek et al. (1994, 1996) advised that for all CV’s \( Pe < 5 \), or at least \( < 10 \), and that \( Co < 1 \). This is in agreement with the Fourier number being less than 0.5 as suggested by Daus et al. (1985). As long as for all nodes these requirements are met, it is believed that numerical dispersion and oscillations are small. No procedure is known to us to completely remove numerical dispersion for two-dimensional models. For implicit, one-dimensional simulations Moldrup et al. (1992, 1994) gave procedures for removing numerical dispersion.

**Dispersion-diffusion**

The dispersive-diffusive parts of \( q_i \), Eq. [142], at the CV interfaces can be obtained from

\[ q_{i,x,i,j}^{d+dt} = - \theta_{z} t \Delta t D_{i,x,i,j}^{t+dt} \frac{c_{i,j+1} - c_{i,j}}{\Delta z_j}, \]

\[ q_{i,z,i,j}^{d+dt} = - \theta_{z} t \Delta t D_{i,z,i,j}^{t+dt} \frac{c_{i,j+1} - c_{i,j}}{\Delta z_j}, \]

\[ q_{i,x,i,j}^{d+dt} = - \theta_{z} t \Delta t D_{i,x,i,j}^{t+dt} \frac{c_{i,j+1} - c_{i,j}}{\Delta z_j}, \]

\[ q_{i,z,i,j}^{d+dt} = - \theta_{z} t \Delta t D_{i,z,i,j}^{t+dt} \frac{c_{i,j+1} - c_{i,j}}{\Delta z_j}. \]

and

\[ q_{i,x,i,j}^{d+dt} = - \theta_{z} t \Delta t D_{i,x,i,j}^{t+dt} \frac{c_{i,j+1} - c_{i,j}}{\Delta z_j}. \]

Note that \( c \) at the nodes from the previous time step are used, while all other quantities refer to the new situation at \( t+\Delta t \). In Eqs. [157] and [158] \( c \) at a node is used, while in Eqs. [159] and [160] \( c \) at an interface between nodes is used. The different components appearing in Eqs. [157]-[160] are given below.

The *dispersion-diffusion coefficients* at the CV interfaces are computed according to Eq. [33], which for two dimensions are given by \((q > 0)\)

\[ \theta D_{xx} = a_1 \frac{q_x^2}{|q|} + a_\tau \frac{q_z^2}{|q|} + \theta D_o \tau(\theta), \]

\[ \theta D_{zz} = a_1 \frac{q_z^2}{|q|} + a_\tau \frac{q_z^2}{|q|} + \theta D_o \tau(\theta), \]

\[ \theta D_{xz} = \theta D_{zx} = (a_1-a_\tau) \frac{q_x q_z}{|q|}. \]
If $q = 0$, then

$$\theta D_{xx} = \theta D_{zz} = \theta D_0 \tau(\theta),$$

$$\theta D_{xz} = \theta D_{zx} = 0.$$  \hspace{1cm} [164]

The water fluxes $q_x$ and $q_z$ needed to compute these coefficients are obtained as follows. The water fluxes perpendicular to the interfaces are known from the water solution procedure, but the water fluxes parallel to the interfaces are computed as the averages of the four nearest available water flux densities in the desired direction. Thus, for a vertical CV interface $q_x$ and $q_z$ are

$$q_x = q_{x,j+1}^{t+\Delta t},$$  \hspace{1cm} [166]

$$q_z = \frac{q_{z,j-1}^{t+\Delta t} + q_{z,j+1}^{t+\Delta t} + q_{z,j+1}^{t+\Delta t} + q_{z,j-1}^{t+\Delta t}}{4}. $$ \hspace{1cm} [167]

For a vertical CV interface $q_x$ and $q_z$ are

$$q_x = \frac{q_{x,j-1}^{t+\Delta t} + q_{x,j+1}^{t+\Delta t} + q_{x,j+1}^{t+\Delta t} + q_{x,j-1}^{t+\Delta t}}{4}, $$ \hspace{1cm} [168]

$$q_z = q_{z,j}^{t+\Delta t}. $$ \hspace{1cm} [169]

The absolute value of the water flux is computed as

$$|q| = \sqrt{q_x^2 + q_z^2}. $$ \hspace{1cm} [170]

In order to **evaluate the dispersive flux in the one direction induced by a gradient in c in the other direction** at a CV interface, the gradient in $c$ along this interface must be estimated (see Eqs. [159] and [160]). The $c$ at the edges of the interfaces, i.e. at the cross points of four CV’s, are computed as the averages of the $c$’s at the four neighbouring CV’s, for example:

$$c_{ij}^t = \frac{c_{ij}^t + c_{i,j+1}^t + c_{i+1,j}^t + c_{i+1,j+1}^t}{4}. $$ \hspace{1cm} [171]

The gradient is the difference in $c$ divided by the length of the interface, with the latter being the width of column or layer.

At the boundaries, the procedure is in principle the same. Dispersive-diffusive components normal to the boundaries are set equal to zero, so that only convective fluxes are present, if any. At a boundary, Eq. [171] reduces to the average of the two nodes at this boundary.

For the special (hypothetical) case $a_p = a_i = 0$, Eq. [33] reduces to

$$\theta D_{ij} = l_p |q| \delta_{ii} + \theta D_0 \tau(\theta) \delta_{ij}, $$ \hspace{1cm} [172]

with $l_p$ being the single dispersivity (L). Equation [172] results only in values for $\theta D_{ii}$ and $\theta D_{ij}$. In the simulation model there is an option to consider a single dispersivity, which requires less computations.
3.4.2 Handling of boundary conditions for solute transport

After the solute flux densities for all interior nodes are computed, the boundary conditions are taken into account. A prescribed concentration at the boundary (Dirichlet condition) means that the solute flux density across the boundary must balance the net solute flux density across the remaining boundaries of that CV (cf. Eqs. [102]-[105]). For example, for a CV at the top the solute flux density across the top boundary, \( q_{xz,i-1,j} \), follows from

\[
q_{xz,i-1} = q_{xz,i} + \left( q_{xz,i} - q_{xz,i-1} \right) \frac{\Delta z_j}{\Delta x_i} + \frac{S_{sij}}{\Delta t \Delta x_i}.
\]  

[173]

Similar equations hold for nodes on other boundaries. Later, when the concentration is computed from Eq. [149], this proper computed solute flux density results in the desired (constant) concentration of that particular boundary node.

The solute flux density across a boundary with a prescribed solute flux density condition (Neumann) is set equal to the desired quantity. The prescribed solute flux density equals the water flux density across the boundary times the proper concentration. Analogously to the upstream weighing method described in Subsection 3.4.1, for an incoming solute the supplied outer concentration is used, while for an outgoing flux the concentration of the CV is used; thus (inflow)

\[
\text{if inflow } q_{s_{i_{\Gamma}}} = q_{\Gamma} c_{\Gamma},
\]  

[174]

where \( c_{\Gamma} \) is the concentration of the incoming water, or (outflow)

\[
\text{if outflow } q_{s_{i_{\Gamma}}} = q_{\Gamma} c_{\Gamma}.
\]  

[175]

A no-flow condition results in a zero solute flux density, i.e. \( q_s = 0 \). In the hypothetical case when no water movement occurs and a fixed concentration at the boundary prevails which is different from the concentration in the soil solution, this will lead to diffusion of solutes towards the lower concentration.

Nodes situated in the CV's at the corners of the flow domain are subject to two boundary conditions. For example, the upper left node is subject to the condition at the surface and at the left boundary. Theoretically, four different situations may exist, since either boundary can be of Dirichlet or Neumann type. In the simulation model care is taken that all possible situations can be dealt with. The Dirichlet and Neumann conditions are treated as described above (see also discussion for water in Subsection 3.2.4).

3.4.3 Root nutrient uptake

In analogy with root water uptake, the root nutrient uptake as described in Chapter 2 (Section 2.6.2) can be used for each control volume. The solution procedure is, however, much simpler than for water uptake. We assume that the root length at each position in the flow domain is known and that all roots potentially can take up at the same rate. Then the required uptake rate per cm root length \( S_{sr} \) (ML^-1T^-1) is

\[
S_{sr,c} = \frac{X Z \Delta y S_{sr}}{\Delta y \sum_{i=1}^{N} \sum_{j=1}^{M} l_{rv_{ij}} \Delta x_i \Delta z_j}.
\]  

[176]

According to Eq. [52], the uptake strength for CV \((i,j)\) is

\[
S_{sij} = \min \left( S_{sr,c} l_{rv_{ij}}, \frac{S_{sm_{ij}}}{\Delta z_j} \right),
\]  

[177]
where the operator min yields the minimum value of its arguments. Roots in favourable situation can compensate for roots in less favourable situation (e.g. De Jager, 1985). So if in some CV's nutrient uptake is limited by the maximum possible uptake, then it is checked whether the remaining CV's can compensate for roots in less favourable conditions.

In short the procedure is as follows. The total available root length is calculated. The maximum uptake rate per CV, $S_{r,\text{un}}$, is computed according to Eq. [50]. Then the actual uptake rate per CV is computed using Eq. [177]. It is checked if the computed uptake rate is physically or physiologically possible: amount taken up may not exceed the amount present corrected for net incoming amount due to solute fluxes across boundaries of CV and it may not exceed any (user supplied) physiologically maximum uptake rate. For each CV it is determined if required uptake can be satisfied. If not, the amount that could not be taken up is temporarily stored. After all CV’s have been considered, the procedure is repeated for all CV’s that could take up at the required rate. Now, the total demand equals the total missing uptake from the previous step per cm root length of the remaining CV’s. The second step may be repeated a third time if in the second step new CV’s cannot take up the new desired amount. These steps are repeated until total uptake equals the required total uptake, or when all CV’s take up at the maximum possible uptake rate.

In the simulation model there is an option to consider root nutrient uptake to occur as nutrient uptake from a CV proportional to root length present in a CV. In analogy with water, Eq. [116], the sink strength term is computed as

$$S_{s,j} = \frac{L_{n,j}}{N \sum_j L_{r,j}} \Delta x_j \Delta z_j S_{s,j}.$$  \[178\]

Of course, the amount taken up from a CV during the time step may not be larger than the amount currently present in the CV.

### 3.5 Time stepping

Computations are carried out for each time step. The time step does not have to be constant. At times when the changes are relatively small larger time steps can be used. In general, one could require that within a time step the change in volumetric water content is restricted. For example, following Vauclin et al. (1979) and Vellidis & Smajstrla (1992) one could choose a new $\Delta t$ which satisfies the condition

$$\Delta t \leq \frac{\zeta \Delta s_{\text{min}}}{| q_{\text{max}} |},$$  \[179\]

where $\zeta$ represents the maximum permissible change in water content during a time step, e.g. $\zeta = 0.01$, $\Delta s_{\text{min}}$ is the minimum grid spacing, and $q_{\text{max}}$ is the magnitude of the maximum net flux into any CV. Note that the net flux of the previous time step is used. Problems may thus occur when boundary conditions change abruptly. Equation [179] is related to the Courant number defined in Eq. [155].

When nutrient transport is included, the time step should also be restricted according to the Courant or Fourier numbers as defined in Eqs. [155] and [156], respectively. According to Daus et al. (1985) $Fo$ should be $\leq 0.5$, so that the time step should meet the restriction

$$\Delta t \leq \frac{(\Delta s_{\text{min}})^2}{2 D_{\text{max}}},$$  \[180\]

where $D_{\text{max}}$ is the maximum observed diffusion/dispersion coefficient in any CV during the current time step.
Care is taken of two possible time events: times of printing, and times when time-dependent boundary conditions change in magnitude such as rain. Since these time events are input, they are known beforehand. The new time step cannot be larger than the difference between time of event and current time.

In summary, the time stepping procedure is as follows. The simulation starts with an initial time step $\Delta t_i$. Each new time step is computed according to

$$ \Delta t = \min(\Delta t_p, \Delta t_r, \Delta t_{\text{te}}, m \Delta t, \Delta t_{\text{max}}, \Delta t_{\text{c}}, \Delta t_f), $$

where $\Delta t_p$ is the time difference between current time and next printing time, $\Delta t_r$ is the time step according to Eq. [179], $\Delta t_{\text{te}}$ is the time difference between current time and next time event due to change in time dependent boundary condition, $m$ is a multiplication factor ($m > 1$), $\Delta t_{\text{max}}$ is a maximum allowable $\Delta t$, $\Delta t_{\text{c}}$ is the required time step based on Co (Eq. [155]), and $\Delta t_f$ is the required time step based on $Fo$ (Eqs. [156] and [181]). If no solute transport is considered $\Delta t_c$ and $\Delta t_f$ are set equal to $\Delta t_{\text{max}}$. During the solution procedure, when no convergence is reached within a maximum number of iterations, $\Delta t$ is reduced by a factor 10. When $\Delta t$ becomes lower than a minimum value $\Delta t_{\text{min}}$ the simulation is halted. Simulations are carried out until $t$ reaches the final time $t_f$. 
4 Hysteretic hydraulic properties

To solve the Richards equation, Eq. [4], for a specific case the hydraulic properties are needed, i.e. the relationships between $K$, $\theta$ and $h$. Several mathematical models have been proposed in the literature. The water retention characteristic is sometimes written as an empirical polynomial or as a nonlinear relationship. In some cases the hydraulic conductivity function is calculated from the water retention characteristic, using assumptions about the pore structure. In soil science the most commonly used models for the hydraulic properties are the models of Van Genuchten (1980) and Mualem (1976). Recently, also the hydraulic properties of some horticultural substrates have been described by these models (e.g. Milks et al., 1980; Wallach et al., 1992a,b; Otten, 1994; Da Silva et al., 1995; Heinem, 1997). We will use these models as well, further referred to as the Van Genuchten-Mualem model (Section 4.1). The $\theta(h)$ and $K(h)$ relationships are known to be hysteretic (Miller & Miller, 1956). In Section 4.2 the modified dependent domain model of Mualem (1984) for describing hysteresis is presented.

4.1 The Van Genuchten-Mualem relationships for $\theta(h)$ and $K(\theta)$

The water retention function $\theta(h)$ given by Van Genuchten (1980) reads as

$$ S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \left\{ \begin{array}{ll} \frac{1}{1 + |a h |^n} & h \leq 0 \\ 1 & h > 0 \end{array} \right. , \quad [182] $$

where $S_e$ is the reduced volumetric water content (-) or effective saturation ($0 \leq S_e \leq 1$), $\theta_r$ and $\theta_s$ are the residual and saturated volumetric water contents (L^-3), respectively, $a$ (L^-1), $n$ ($n > 1$; (1)) and $m$ (1) are curve shape parameters. The steepness of the water retention characteristic is determined by $n$, whereas $m$ determines the value for $S_e$ when $h = -1/a$. For given constant parameters, an increase in $a$ causes a shift of the water retention characteristic to lower volumetric water contents.

The hydraulic conductivity function $K(\theta)$ given by Mualem (1976) reads as

$$ K_e(S_e) = \frac{K(S_e)}{K_s} = \left[ \frac{s_e^a}{\frac{1}{\int_0^s h^{-1}(\eta) \, d\eta}} \right]^{2} , \quad [183] $$

where $K_s$ is the relative hydraulic conductivity (1), $K_e$ is the hydraulic conductivity (LT^-1) at saturation, and $a$ is a curve shape parameter (1) representing a pore-size distribution index, which is sometimes assumed to be equal to 0.5 as suggested by Mualem (1976). For saturated conditions, i.e. $h = 0$, $S_e = 1$ (Eq. [182]), Eq. [183] reduces to $K_e(1) = 1$. Substituting Eq. [182] in Eq. [183] one obtains (Leij et al., 1992)

$$ K_e(S_e) = S_e^2 \left[ l_{se}^{m+1/n, 1-1/n} \right]^{2} , \quad [184] $$

where $l_{se}$ is the incomplete beta function of order $\eta$. In case the parameters $m$ and $n$ are related according to
\[ m = 1 - \frac{1}{n}, \quad n > 1, \quad [185] \]

a simple expression for \( K_r \) is obtained

\[ K_r(S_e) = S_e^\prime \left[ 1 - \left( 1 - S_e^{\text{lim}} \right)^m \right]^2. \quad [186] \]

The corresponding expression for \( K_r(h) \) follows from substitution of Eq. [182] in Eq. [186]:

\[ K_r(h) = \begin{cases} \frac{[(1 + |ah|^n)^m - |ah|^{n-1}]^2}{(1 + |ah|^n)^{(d+2)m}} & h \leq 0, \\ 1 & h > 0. \end{cases} \quad [187] \]

Finally, substituting Eq. [182] in Eq. [6], an expression for the differential moisture capacity \( C(h) \) can be obtained:

\[ C(h) = \begin{cases} (\theta_c - \theta_r) n m a^n |h|^{n-1}(1 + |ah|^n)^{-1-m} & h \leq 0, \\ 0 & h > 0. \end{cases} \quad [188] \]

Standard laboratory techniques are available to determine the water retention and hydraulic conductivity characteristics. Parameter optimization programs are available to obtain estimates for the parameters in the Van Genuchten-Mualem model. Examples of such programs are: RETC (Van Genuchten et al., 1991; Leij et al., 1992), SFIT (Kool & Parker, 1987a), MULSTP (Van Dam et al., 1994), and MLSTPM (Eching et al., 1994). Existing mathematical software packages can also be used to obtain parameter estimates, e.g. Heinen (1997) used Mathematica (Wolfram, 1991) to obtain simultaneously the Van Genuchten parameters for the drying and wetting data.

### 4.2 Modified dependent domain hysteresis model of Mualem

The relationships \( \theta(h) \) and \( K(h) \) are known to be hysteretic (Miller & Miller, 1956), which means that different relationships exist for drying and wetting processes. It is assumed that \( K(\theta) \) is not hysteretic. Topp (1969) showed experimentally that \( \theta(h) \) is hysteretic and that \( K(\theta) \) has negligible hysteresis. Any porous medium has hysteretic hydraulic properties. Following Kool & Parker (1987b), in this report we use the following hysteresis model.

#### The main drying and wetting water retention curves

The main drying water retention characteristic can be expressed by Eq. [182], with the parameters:

\[ \theta_{c,d}, \quad \theta_{r,d}, \quad \alpha_d, \quad n_d, \quad m_d, \]

and the main wetting water retention characteristic can also be expressed by Eq. [182], with the following parameters:

\[ \theta_{c,w}, \quad \theta_{r,w}, \quad \alpha_w, \quad n_w, \quad m_w. \]

The subscripts \( d \) and \( w \) refer to main drying and main wetting, respectively. In order to reduce the number of parameters, following Kool & Parker (1987b), it is assumed that
\[ \theta_{sd} = \theta_{sw} = \theta_s, \quad \theta_{oh} = \theta_{ow} = \theta_o, \quad n_d = n_w = n, \text{ and } m_d = m_w = m. \]

This implies that the main wetting characteristic and the main drying characteristic only differ in the parameter \( \alpha \). For \( \alpha_w > \alpha_d \) the wetting curve lies to the left of the drying curve. The two main curves are closed at the end-points \( \theta_s \) and \( \theta_o \). Note that the main wetting characteristic also ends at \( \theta_s \), implying that air entrapment, at \( h = 0 \), is not taken into account.

In case the drying process along the main drying curve is reversed into a wetting process somewhere in the flow domain, then a scanning wetting curve is followed. Similarly, scanning drying curves exist. Between the main wetting characteristic and the main drying characteristic there are an infinite number of scanning curves. It is time-consuming to determine a large number of scanning curves in the laboratory, so that mathematical models are very useful. With these models the scanning curves can be computed. It is important that such a model considers scanning curves as closed loops, otherwise the so-called pumping effect (Jaynes, 1984) occurs. Comparisons of several hysteresis models were carried out by Jaynes (1984) and Viaene et al. (1994). In this report the modified dependent domain model of Mualem (1984), having closed scanning loops, is used. In a comparative, statistical study by Viaene et al. (1994), this model performs best of the so-called two-branch models. Two-branch hysteresis models require as input both the main drying and the main wetting characteristics. The expressions for the scanning curves are given below using the notation used by Kool & Parker (1987b).

**Modified dependent domain model of Mualem (1984)**

Mualem’s (1984) model accounts for the pore water blockage against air in drying processes, but blockage of access to water during wetting processes is considered negligible. Thus the dependence of the domains refers to the drying process, and in the wetting process the pores are assumed to be independent. This results in a complicated expression for drying and a simpler one for wetting. The scanning drying curve is defined as (Fig. 7)

\[ \theta_{sd}(h) = \theta_s - P(\theta)[\theta_s - \theta_{sw}(h)][\theta_{w}(h_d) - \theta_{w}(h)], \tag{189} \]

and the scanning wetting curve is defined as (Fig. 7)

\[ \theta_{sw}(h) = \theta_s + P(\theta)[\theta_s - \theta_{sw}(h_d)][\theta_{w}(h) - \theta_{w}(h_d)], \tag{190} \]

where subscripts \( sw \) and \( sd \) refer to the scanning wetting and scanning drying curves, respectively, and subscript \( d \) refers to the reversal point. The different components of Eqs. (189) and (190) are shown in Fig. 7.

The function \( P(\theta) \) is given by

\[ P(\theta) = \frac{\theta_s - \theta}{[\theta_s - \theta_{w}(h^*)]^2}, \tag{191} \]

where \( h^* \) is the pressure head at which

\[ \theta_{sd}(h^*) = \theta. \tag{192} \]

Using Eq. (182) \( h^* \) can be computed as follows\(^4\)

\[ h^* = -\frac{1}{\alpha_d} \left[ \left( \frac{\theta - \theta_s}{\theta_s - \theta_o} \right) \right]^{-1/m} \left[ \left( \frac{\theta - \theta_s}{\theta_s - \theta_o} \right) - 1 \right]^{1/n}. \tag{193} \]

For drying processes \( P \) is a function of the unknown \( \theta \), while for wetting processes \( P \) is a function of the known \( \theta_s \). Therefore, Eq. (189) must be solved iteratively, while Eq. (190) can be computed directly. A short discussion on the function \( P \) is presented in the Appendix 2. For a further

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\(^4\) *Note that in Eq. (11) of Kool & Parker (1987b) the minus sign is missing.*
Figure 7  Main drying, main wetting, and examples of scanning drying (A) and scanning wetting (B) curves according to Eqs. [189] and [190], respectively. Parameter values apply to a mixture of 75% peat and 25% perlite (hydraulic properties from Otten, 1994).
discussion on the function \( P \) the reader is referred to Mualem (1984).

The Mualem model fails to converge to the correct \( \theta_i \) or \( \theta_e \). Therefore, an additional constraint is needed to prevent \( \theta \) falling outside the main wetting curve and main drying curve:

\[
\theta_w(h) \leq \theta(h) \leq \theta_d(h).
\]  

[194]

The *differential moisture capacity belonging to the drying scanning curve* follows from differentiating Eq. [189] with respect to \( h \):

\[
C_{sd}(h) = (T_1 + T_2)P(\theta)[1 + T_1 T_2 T_3]^{-1} C_w(h),
\]

[195]

with

\[
T_1 = \theta_e - \theta_w(h),
\]

[196]

\[
T_2 = \theta_w(h_d) - \theta_w(h),
\]

[197]

and

\[
T_3 = \left[ \frac{\theta_s - \theta_w(h^*)}{\theta_s - \theta_w(h)} \right]^{-2} + 2 \left( \theta_s - \theta \right) \left[ \frac{\theta_s - \theta_w(h^*)}{\theta_s - \theta_w(h)} \right]^{-1} T_4 C_w(h^*),
\]

[198]

with

\[
T_4 = \left[ \alpha_d(n-1)(\theta - \theta_i) \right]^{-1} \left[ \frac{\theta - \theta_i}{\theta_s - \theta_i} \right]^{-m} - 1 \left[ \frac{\theta - \theta_i}{\theta_s - \theta_i} \right]^{-1/m}.
\]

[199]

The *differential moisture capacity belonging to the wetting scanning curve* follows from differentiating Eq. [190] with respect to \( h \):

\[
C_{sw}(h) = P(\theta_d)\left[ \frac{\theta_s - \theta_w(h_d)}{\theta_s - \theta_w(h)} \right] C_w(h).
\]

[200]

A complicated expression for the drying differential moisture capacity, i.e. Eq. [195], is obtained due to differentiating \( P \) with respect to \( h \), while for the wetting process the derivative \( \partial P/\partial h \) is zero, and thus a simple expression for \( C_{sw} \), i.e. Eq. [200], is obtained.

For each grid point in the control volume model (see Chapter 3) the hysteresis model must be used. Thus for each node the status of drying or wetting must be known and adapted if necessary. The status of the node is stored as \( \kappa_n \) and can have four values:

-2: drying along main drying curve,
-1: drying along scanning drying curve,
+1: wetting along scanning wetting curve, and
+2: wetting along main wetting curve.

A change of \( \kappa_n \) occurs when \( h \) at a node at time \( t+\Delta t \) meets the criterion (Kool & Parker, 1987b)

\[
\frac{h^* - h}{\kappa} \geq \epsilon_\kappa,
\]

[201]

where \( \epsilon_\kappa \) is set to some small positive number, e.g. \( \epsilon_\kappa = 0.01 \), to ignore the effect of small local oscillations in the calculated pressure head, and \( \kappa \) is defined as

\[\text{Note that they used } -T_2 \text{ in the expression for } T_1 \text{ and that in } T_4 \text{ the term } (1-n) \text{ was used. This is the same as } +T_4 \text{ with in the expression for } T_1 \text{ the term } (n-1) \text{ as is given here.}\]

\[\text{Eq. (14) of Kool & Parker (1987b) is wrong. They gave a minus-sign in front of } T_1 T_2 T_3 \text{ instead of a plus-sign. In the expression for } T_1 \text{ they raised the term between square brackets to the power } +m \text{ instead of } -m. \text{ The parameter } \alpha \text{ was not specified as } \alpha_d.\]

\[\text{Note that they used } -T_2 \text{ in the expression for } T_1 \text{ and that in } T_4 \text{ the term } (1-n) \text{ was used. This is the same as } +T_4 \text{ with in the expression for } T_1 \text{ the term } (n-1) \text{ as is given here.}\]
\[ \begin{align*}
\kappa^* &= -1 \quad \text{if } \kappa_h < 0 \\
\kappa^* &= +1 \quad \text{if } \kappa_h > 0
\end{align*} \] [202]

Possible reversals of \( \kappa_h \) are from \(-2\) or \(-1\) to \(+1\), from \(+2\) or \(+1\) to \(-1\), from \(-1\) to \(-2\), and from \(+1\) to \(+2\). The change from \(-1\) to \(-2\) or from \(+1\) to \(+2\) occurs when the constraint of Eq. [194] is not met. As soon as the status of a node becomes \(+2\) or \(-2\) Eqs. [182] and [187] (Section 4.1) can be used.

Note that, after returning at a reversal point, the Musalem hysteresis model stays on the current scanning loop. Other models (Dirksen et al., 1993; Otten, 1994) step over on the previous scanning loop. A comparison between the hysteresis module described here and that of Dirksen et al. (1993) yielded similar results for some one-dimensional flow problems (Koorevaar, 1995, pers. comm.).
5 User's guide

5.1 Model structure

The numerical model presented in Sections 3.2 - 3.5 was programmed in Fortran 77. An early version of the model was described by Heinen & De Willigen (1992), in which only the ADI method was used and in which no solute transport and root uptake was considered. A simplified flow scheme of the sequential computations is given in Fig. 8. In the main program (Fig. 8A) the respective computations are carried out in a time-loop until the final time $t_f$ is reached. The equations that are used are given between square brackets in Fig. 8. By setting switches in a control file, root water uptake, solute transport and root nutrient uptake can be included or excluded. It is assumed that when solute transport is considered water movement is considered as well, and that when root nutrient uptake is considered, root water uptake is also considered. The core of the simulation model is the module that solves the Richards equation (Fig. 8B). In a iteration loop the solution is obtained either through the ADI method or the ICCG method. If convergence problems arise (maximum number of iterations exceeded, or $\Delta t$ becomes too large) the time step is decreased and the iterations are started again beginning with the values of $h^i$, $\theta^i$, $K^i$, and $C^i$. The computations of the new status variables ($\theta_{n+1}^i$, $K_{n+1}^i$, and $C_{n+1}^i$) for ADI also $\theta_{n+1/2}^i$, $K_{n+1/2}$, and $C_{n+1/2}$) including hysteresis are done according to the models presented in Chapter 4. When convergence is reached the Darcian flux densities across the CV interfaces in x- and z-directions are computed according to Eqs. [100]-[105]. They can be used to generate flux density distribution plots (see e.g. Heinen, 1997), and they are used in the solute transport module. There are also routines for writing output to files and for computing integral properties, such as net amounts of input into flow domain (not shown in Fig. 8).

5.2 Correspondence between variables in files and variables in text

Table 3 lists the input parameters required by the simulation model, and of the (possible) output variables. Table 4 summarizes the correspondence between the names of variables in the different input files and the variables used in the text of this report.

Each printing time the following general information is written to the output file (see Section 5.4 for examples of output files).

**Water**
- Total amount of water present in the flow domain, being the summed amounts present in each CV which is the volumetric water content in the CV times the volume of the CV (ml).
- The total change of water in the flow domain since $t = 0$, which is due to net inflow of water across the boundaries (ml).
- The water balance error in absolute sense, defined as the current water storage minus the initial water storage minus the total change (ml).
- The relative balance error defined as the water balance divided by the current water storage.
- The net amount that has entered the flow domain since $t = 0$ across each of the four boundaries.

**Solute**
- Total amount of solute(s) present in the flow domain, being the summed amounts present in each CV (mmol).
- The total change of solute(s) in the flow domain since $t = 0$, which is due to net inflow of solute(s) across the boundaries (mmol).
- Total solute uptake of solute(s) by the crop since $t = 0$ (mmol)
- The solute(s) balance error(s) in absolute sense, defined as the current solute(s) storage minus the initial solute(s) storage minus the total change of solute(s) (mmol).
- The relative balance error(s) defined as the balance divided by the current storage.
- The net amount that has entered the flow domain since $t = 0$ across each of the four boundaries.
(A) Flow scheme indicating sequence of main computations in simulation model and (B) detail of sequence of computations for solving the Richards equation. Reference to equation numbers in the text are given in square brackets.
Table 3  Lists of input parameters required by the simulation model, and list of (possible) output variables which are given at user-supplied print times.

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<th>Input parameters</th>
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<tbody>
<tr>
<td><strong>Water</strong></td>
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</tr>
<tr>
<td>$N$, $M$, $\Delta X_u$, $\Delta Z$,</td>
<td></td>
</tr>
<tr>
<td>For all $(i,j)$: $\theta_{i,j}$, $n_{i,j}$, $a_{i,j}$, $a_{w}$, $K_r$, $\lambda$</td>
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</tr>
<tr>
<td><strong>Top boundary conditions</strong></td>
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<td>$h_{\max}(i)$, $\Delta t_{\max}$, $\Delta t_{\text{min}}$, $t_p$, $z$, $t_m$</td>
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</tr>
<tr>
<td>$\epsilon$, $\epsilon_0$, maximum number of iterations</td>
<td></td>
</tr>
<tr>
<td>Initial $x_{i,j}$, $x_{i,j}$ (see Chapter 4)</td>
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</tr>
<tr>
<td><strong>Root water uptake</strong></td>
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</tr>
<tr>
<td>$K_r$, $R_{\text{w}}$, $a$, $h_{\text{w}}$, $z$</td>
<td></td>
</tr>
<tr>
<td>$L_{\text{w}}(i,j)$ (if root growth give also $k_{i,j}$, $t^*$ and start time, and $L_{\text{w}}(i,j) = L_{\text{w}}(i,j)$, see Chapter 7 of Heinen, 1997)</td>
<td></td>
</tr>
<tr>
<td><strong>Solute transport</strong></td>
<td></td>
</tr>
<tr>
<td>$c_{i,j}$, $a_{i,j}$, $D_{\text{w}}$, $f_{i,j}$, $f_{i,j}$, $\theta(i,j)$</td>
<td></td>
</tr>
<tr>
<td>$c_{i,j}(i,j)$</td>
<td></td>
</tr>
<tr>
<td><strong>Root nutrient uptake</strong></td>
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</tr>
<tr>
<td>$S_{\text{u}}$</td>
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</tr>
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<table>
<thead>
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<th>Output variables (per printing time)</th>
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<td>$\theta(i,j)$, $h(i,j)$, $K(i,j)$, $C(i,j)$, $H(i,j)$, $q_{i,j}$, $q_{w}(i,j)$</td>
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</tr>
<tr>
<td>$\theta(i,j)$, $h(i,j)$, $k(i,j)$, $q_{w}(i,j)$, $q_{w}(i,j)$</td>
<td></td>
</tr>
<tr>
<td><strong>Root water uptake</strong></td>
<td></td>
</tr>
<tr>
<td>$S_{\text{u}}(i,j)$ (actual rate and cumulative since $t = 0$), $h_{\text{u}}$, $T$, total water uptake by plant roots</td>
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</tr>
<tr>
<td><strong>Nutrient transport</strong></td>
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</tr>
<tr>
<td>$c(i,j)$, $Q_{i,j}$, $q_{i,j}$, $q_{w}(i,j)$</td>
<td></td>
</tr>
<tr>
<td>$c(i,j)$, $Q_{i,j}$, $q_{i,j}$, $q_{w}(i,j)$</td>
<td></td>
</tr>
<tr>
<td><strong>Root nutrient uptake</strong></td>
<td></td>
</tr>
<tr>
<td>$S_{\text{u}}(i,j)$ (actual rate and cumulative since $t = 0$), total nutrient uptake by plant roots</td>
<td></td>
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</table>
Table 4  Correspondence between variables used in input files and variables used in text with reference to equation of first occurrence in text or section of description (continued on next pages), and indication of type of variable (real (double precision), integer, character), dimension of variable (with t indicating the user-supplied time units UNITS), and number of array entries required. Data are grouped per input file, and only most important variables are listed. Input files are described in more detail in Section 5.3.

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<th>Variable names in input files</th>
<th>Type of variable</th>
<th>Number of array entries</th>
<th>Variables used in text</th>
<th>Dimension</th>
<th>Equation Section</th>
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<td>[95], [96]</td>
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<td>( L )</td>
<td></td>
<td></td>
<td>[181]</td>
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<td>( m_r )</td>
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<td>( \Delta t_{\text{mile}} )</td>
<td>( t )</td>
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<td>[133], [134]</td>
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<td>the factor 100 in the denominator of Eqs. [133] and [134]</td>
<td>cm (Eq. [133]) or cm ( t^4 ) (Eq. [134])</td>
<td>[133], [134]</td>
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<td>[219,220]</td>
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<td>[218,220]</td>
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*filnam* (Section 5.3.3)

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<td>cm$^3$ cm$^{-3}$</td>
<td>[182]</td>
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<td>cm$^{-1}$</td>
<td>[182]</td>
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*bname.DAT* (Section 5.3.4)

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<td>$h_r$</td>
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<td>$q_t$</td>
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<td>NL</td>
<td>$q_r$</td>
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<td>Unit</td>
<td>Notes</td>
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### wname.DAT (Section 5.3.6)

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<td>real</td>
<td>$q_{ir}$</td>
<td>cm t$^{-1}$</td>
<td>[10,5.3.2]</td>
</tr>
<tr>
<td>LFRAC</td>
<td>real</td>
<td></td>
<td></td>
<td>5.3.2</td>
</tr>
<tr>
<td>ETPTH</td>
<td>real</td>
<td></td>
<td>cm t$^{-1}$</td>
<td>5.3.2</td>
</tr>
<tr>
<td>HTRESH</td>
<td>real</td>
<td></td>
<td>cm</td>
<td>5.3.2</td>
</tr>
<tr>
<td>ECTRSH</td>
<td>real</td>
<td></td>
<td>dS m$^{-1}$</td>
<td>5.3.2</td>
</tr>
<tr>
<td>JTRESH</td>
<td>integer</td>
<td></td>
<td></td>
<td>5.3.2</td>
</tr>
</tbody>
</table>

### transp.DAT (Section 5.3.7)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Type</th>
<th>Description</th>
<th>Unit</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIGMA</td>
<td>real</td>
<td>$\sigma$</td>
<td></td>
<td>[20]</td>
</tr>
<tr>
<td>HOSP</td>
<td>real</td>
<td>$h_{u,v}$</td>
<td>cm</td>
<td>[20]</td>
</tr>
<tr>
<td>K1</td>
<td>real</td>
<td>$K_1$</td>
<td>cm d$^{-1}$</td>
<td>[20]</td>
</tr>
<tr>
<td>R0</td>
<td>real</td>
<td>$R_0$</td>
<td>cm</td>
<td>[21]</td>
</tr>
<tr>
<td>REDPOT</td>
<td>integer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>---------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>real</td>
<td>$a$</td>
<td>[26]</td>
<td></td>
</tr>
<tr>
<td>HRHALF</td>
<td>real</td>
<td>$h_{r,1/2}$</td>
<td>[26]</td>
<td></td>
</tr>
<tr>
<td>LRVINI</td>
<td>real</td>
<td>NL*NC $L_0(t=0)$</td>
<td>cm cm$^3$</td>
<td>[19]</td>
</tr>
<tr>
<td>RTGROW</td>
<td>integer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LRVK</td>
<td>real</td>
<td></td>
<td>[203]</td>
<td></td>
</tr>
<tr>
<td>LRVTS</td>
<td>real</td>
<td></td>
<td>[203]</td>
<td></td>
</tr>
<tr>
<td>LRVT</td>
<td>real</td>
<td></td>
<td>[203]</td>
<td></td>
</tr>
<tr>
<td>OUTTRA</td>
<td>integer</td>
<td>4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**TRANS.PCTR (Section 5.3.8)**

<table>
<thead>
<tr>
<th>TRANS</th>
<th>character*7</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAC</td>
<td>real</td>
</tr>
<tr>
<td>RDPMIN</td>
<td>real</td>
</tr>
<tr>
<td>NP</td>
<td>integer</td>
</tr>
<tr>
<td>TOL</td>
<td>real</td>
</tr>
<tr>
<td>TRHYST</td>
<td>character*1</td>
</tr>
</tbody>
</table>

**TGEN.DAT (Section 5.3.9)**

<table>
<thead>
<tr>
<th>NNTAB</th>
<th>integer</th>
</tr>
</thead>
<tbody>
<tr>
<td>PPBIG</td>
<td>real</td>
</tr>
<tr>
<td>PPREF</td>
<td>real</td>
</tr>
<tr>
<td>PPEND</td>
<td>real</td>
</tr>
</tbody>
</table>

**facil.DAT (Section 5.3.10) below NION (≤ 13) represents the number of ions present in solution**

<table>
<thead>
<tr>
<th>JSTOP, IBOT</th>
<th>integer</th>
<th>NC</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTOP, CBOT</td>
<td>real</td>
<td>NION*NC $c_T$ mmol</td>
</tr>
<tr>
<td>JLEFT, JRIGHT</td>
<td>integer</td>
<td>NL</td>
</tr>
<tr>
<td>CLEFT, CRIGHT</td>
<td>real</td>
<td>NION*NL $c_T$ mmol</td>
</tr>
<tr>
<td>FREQF</td>
<td>integer</td>
<td></td>
</tr>
<tr>
<td>IDISP</td>
<td>integer</td>
<td></td>
</tr>
<tr>
<td>LD</td>
<td>real</td>
<td>$L_0$ cm</td>
</tr>
<tr>
<td>AL</td>
<td>real</td>
<td>1 or NL*NC $a_i$ cm</td>
</tr>
<tr>
<td>AT</td>
<td>real</td>
<td>1 or NL*NC $a_r$ cm</td>
</tr>
<tr>
<td>CF1</td>
<td>real</td>
<td>NL*NC $f_i$</td>
</tr>
<tr>
<td>CF2</td>
<td>real</td>
<td>NL*NC $f_2$</td>
</tr>
<tr>
<td>WCLOW</td>
<td>real</td>
<td>NL*NC $\theta_i$ cm$^3$ cm$^{-3}$</td>
</tr>
<tr>
<td>ICON</td>
<td>integer</td>
<td></td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th>CONC</th>
<th>real</th>
<th>NION<em>NL</em>NC</th>
<th>C</th>
<th>mmol l⁻¹</th>
<th>[45]</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMOUNT</td>
<td>real</td>
<td>NION<em>NL</em>NC</td>
<td>Qₘₐ</td>
<td>mmol or mg</td>
<td>[46]</td>
</tr>
<tr>
<td>OUTSLT</td>
<td>integer</td>
<td></td>
<td>7</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**IONSINFO.DAT** (Section 5.3.11)

| IONYES | integer | 13     |       |         |      |
| IONNAM | character*5 | 13     |       |         |      |
| MOBIL  | real | 13     | μₘₐ   | cm s⁻¹ V⁻¹ | [35], [43] |
| IONRAD | real | 13     | dᵢ    | Ångstrom | [37] |
| VALENC | real | 13     | nᵦ   |         | [35], [36], [37], [43] |
| DIF0   | real | 13     | Dₒ    | cm² d⁻¹ | [33], [43] |
| DEBYE  | integer |       |       |         |      |
| PARAB  | integer |       |       |         |      |
| PARA   | real | 13     | Aᵦ   | (mol kg⁻¹)⁷⁶⁶ | [38] |
| PARB   | real | 13     | Bᵦ   | (mol kg⁻¹)⁷⁶⁶ m⁻¹ | [39] |

**UPTA.DAT** (Section 5.3.12)

| IUPWAY | integer |       |       |         |      |
| IUPMAX | integer |       |       |         |      |
| UPCRIT | real |       |       |         |      |
| METHOD | integer |       |       |         |      |
| NPLANT | integer |       |       |         |      |
| PLUPT  | real | 13     | Sᵦₚ  | mmol d⁻¹ | [51] |
| FMAX   | real | 13     |       |         | 3.4.3 |

### 5.3 Detailed description of input files

The program FUSSIM2 needs a total of 12 input files (maximum): 6 files are user-supplied file names (with a default extension .DAT), and 6 files are default file names, i.e. INPUT.DAT, FUS2.CTR, TRANSN.CTR, TGEN.DAT (if transpiration is considered), IONSINFO.DAT (if solute transport is considered) and UPTA.DAT (if solute uptake is considered). The structures of all input files are described below. Under very special conditions other files may be required as well, which is mentioned at the descriptions below (WET.DAT, THHFXFZ.DAT).

In general, the input files have the following structure

```
VARIABLE = <value>
```

where VARIABLE is a defined variable name which cannot be altered by the user. Behind the equal sign the value(s) for that variable name are listed: a single value or a character string, or an array of values. This kind of input is regulated by the TTUTIL library of Rappoldt & Van Kraalingen (1990). The rules are:
- no more than 80 characters per line; if more positions are needed just continue on next line;
- array elements should be separated by a space or a comma;
• repeated similar elements in an array may be indicated as n*value, e.g. 16*10.0, 5*2.0 (21 elements in total);
• character data must be given in single quotes;
• integer values must be given as integers;
• real values must be given as reals;
• position of variable name in data file is free;
• extra variable names may be present;
• information behind a * or a ! is considered as comment, and is not read by the program.

Any violation of these rules is properly echoed to the screen followed by a halt of program execution. Moreover, in several cases additional checks on the data are done in the program, such as check on proper amount of supplied array elements. Mostly, the description in the example files given below is self-explanatory. In some cases some additional information on a specific variable is given. In Table 4 the correspondence between the variable names in the files and the variable names used in the text is given. Table 5 gives the maximum values or number of array elements for some variables.

Table 5  Maximum value or maximum number of array elements for several variables.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Maximum value</th>
<th>Maximum number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>NC</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>NL</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>RAIN</td>
<td></td>
<td>20000</td>
</tr>
<tr>
<td>EPOT</td>
<td></td>
<td>20000</td>
</tr>
<tr>
<td>TPOT</td>
<td></td>
<td>20000</td>
</tr>
<tr>
<td>PRTIME</td>
<td></td>
<td>400</td>
</tr>
<tr>
<td>NSOILS</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>NSEEP</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>JSEEP?</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>JSEEP?</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>XWET</td>
<td></td>
<td>50</td>
</tr>
<tr>
<td>YWET</td>
<td></td>
<td>50</td>
</tr>
<tr>
<td>NION</td>
<td></td>
<td>13</td>
</tr>
</tbody>
</table>

5.3.1 Input file INPUT.DAT

The file INPUT.DAT (example in Table 6) contains the 6 user-supplied input filenames and the 2 user-supplied output filenames. The names TRANSP is required if root water uptake is considered and the names FLSALT and SLTNAM are required if solute transport is considered. In case root water uptake is considered the files TRANSP.CTR and TGEN.DAT must be present in the current directory, and when root solute uptake is considered the file UPTA.DAT must be present in the current directory. The structure of all input files, using the names as specified in INPUT.DAT, are described below.

Table 6  Example input file INPUT.DAT.

```
SNAME = 'soil'           ; Name of soil data input file
BNAME = 'bounds'         ; Name of boundary conditions input file
TNAME = 'timer'          ; Name of timer data input file
WNAME = 'weather'        ; Name of weather data input file
TRANSP = 'transp'        ; Name of transpiration data input file
FLSALT = 'solute'        ; Name of solute data input file
```
RNAME = 'outwat'  ! Name of water output file
SLTNAM = 'outslt'  ! Name of solute output file

5.3.2 Input file FUS2.CTR

The file FUS2.CTR (example in Table 9) contains some control data used by the program. Some of the data can be safely adapted by the user, while others are preferred not to be changed by the user (reason: requires too much inside information in the model, or not thoroughly tested by the developers). The variables that should not be changed are: DUMP, PRTINY, TOODEV, BIG, KHFACX, KHFACZ, BOTIRR.

STSTAT
Transport under steady state conditions can be considered as follows; for example, if one is interested in solute transport under steady water flow. First make a run for water only for a long period and determine the steady state situation. If steady state is reached make a file (using the proper output data from these computations) named THHFXFZ.DAT (example in Table 7) in which the following information is stored: (per control volume) water content, pressure head, flux density in x direction, and flux density in z direction. Then, run the model with STSTAT="Y" for the situations to be considered. No computations for water flow will be carried out, since water content, pressure head, and flux densities are considered constant.

Table 7 Example of file THHFXFZ.DAT (NC = 3, NL = 3; fictive data). Note that for flux in x direction NC+1 data are needed, and for flux in z direction NL+1 data are needed.

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.2</td>
<td>0.25</td>
</tr>
<tr>
<td>0.25</td>
<td>0.25</td>
<td>0.3</td>
</tr>
<tr>
<td>0.3</td>
<td>0.31</td>
<td>0.35</td>
</tr>
<tr>
<td>-100.</td>
<td>-100.</td>
<td>-95.</td>
</tr>
<tr>
<td>-95.</td>
<td>-95.</td>
<td>-80.</td>
</tr>
<tr>
<td>-80.</td>
<td>-78.</td>
<td>-50.</td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>-0.1</td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>-0.12</td>
</tr>
<tr>
<td>0.0</td>
<td>-0.01</td>
<td>-0.2</td>
</tr>
<tr>
<td>-0.05</td>
<td>-0.05</td>
<td>-0.05</td>
</tr>
<tr>
<td>-0.05</td>
<td>-0.05</td>
<td>-0.05</td>
</tr>
<tr>
<td>-0.05</td>
<td>-0.05</td>
<td>-0.05</td>
</tr>
</tbody>
</table>

METHIR
The model has several possibilities to control water supply at the top boundary.

METHIR = 0 User supplied times and intensities of rainfall or irrigation; data in file WNAME (default).

METHIR = 1 Program 'controls' irrigation: water is supplied whenever a threshold value for summed potential evapotranspiration is reached. The user supplies in the file WNAME the necessary information, which is:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>IRRINT</td>
<td>irrigation intensity (cm per time units)</td>
</tr>
<tr>
<td>ETPTH</td>
<td>threshold evapotranspiration (cm)</td>
</tr>
<tr>
<td>LFRAC</td>
<td>leaching fraction, defined as the excess amount of water to be supplied, i.e. amount of water supplied is (1+LFRAC)*ETPTH (this is not the usual definition of leaching fraction (LF); Heinen (1997) gives the relation between LFRAC and LF: LF=LFRAC/(1+LFRAC), or LFRAC = LF/(1-LF))</td>
</tr>
</tbody>
</table>

METHIR = 2 Program 'controls' irrigation: water is supplied whenever the pressure head at a given position becomes less (more negative) than a given threshold value. The user supplies in the file WNAME the necessary information, which is:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>IRRINT</td>
<td>irrigation intensity (cm per time units)</td>
</tr>
</tbody>
</table>
| LFRAC | leaching fraction, defined as the excess amount of water to be
supplied, i.e. amount of water supplied is \((1 + LFRAC) \times ETPTH\) (see above).

**HTRESH**  threshold value of pressure head (cm)

**ITRESH**  column number of node at which pressure head is to be controlled

**JTRESH**  row number of node at which pressure head is to be controlled

If either **ITRESH** or **JTRESH** equals zero, the program checks the complete flow domain for any pressure head being less than **HTRESH**.

**METHIR = 3**

Program 'controls' irrigation: water is supplied whenever the electrical conductivity at a given position becomes larger than a given threshold value. The user supplies in the file **WNAME** the necessary information, which is:

**IRRINT**  irrigation intensity (cm per time units)

**LFRAC**  leaching fraction, defined as the excess amount of water to be supplied, i.e. amount of water supplied is \((1 + LFRAC) \times ETPTH\) (see above)

**ECTRSH**  threshold value of electrical conductivity (dS m\(^{-2}\))

**ITRESH**  column number of node at which electrical conductivity is to be controlled

**JTRESH**  row number of node at which electrical conductivity is to be controlled

If either **ITRESH** or **JTRESH** equals zero, the program checks the complete flow domain for any electrical conductivity being larger than **ECTRSH**.

**WET**

If hysteresis is to be considered the wetting data are described by the Van Genuchten equation, with \(\alpha_w\) (WET = 'GENUCHT'; default). However, it is possible to represent the wetting curve also by tabulated data. In that case intermediate data are obtained either through linear interpolation (WET = 'LINEAR') or through cubic spline interpolation (WET = 'SPLINE'). The tabulated data have to be supplied in an additional file called WET.DAT (example in Table 8).

**Table 8**  Example of a file WET.DAT.

<table>
<thead>
<tr>
<th>XWET</th>
<th>YWET</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0, 0.1, 0.2, 0.5, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 1.00</td>
<td>0.0, 0.025</td>
</tr>
</tbody>
</table>
5.3.3 Input file SOIL.DAT

In this input file general information about the flow domain is given (example in Table 11), such as soil type, number and thickness of columns, and number and thickness of rows.

INSIDE
Variable INSIDE indicates which of the NL*NC nodes are inside the flow domain. The data NC and NL define the maximum rectangular extension of the flow domain. Setting INSIDE = 0 for some nodes, these nodes are not considered in the computations. In this way the actual irregular boundaries can be handled. See example 6.4.

CTREAT
The variable CTREAT determines how the hydraulic conductivity is considered: computed according to the Van Genuchten-Mualem model (CTREAT = 0; default), computed according to the exponential K(h) relationship of Gardner (1958) (CTREAT = 1; used in example 6.2), or treated as a constant (CTREAT = 2; used in example 6.1). In case CTREAT = 1, the parameter in the exponential expression becomes equal to the \( \alpha \) given in the Van Genuchten table. In case CTREAT = 2 the constant hydraulic conductivity (CONCON) and constant differential moisture capacity should be supplied (CONCAP).

FILNAM
The file FILNAM contains the Van Genuchten-Mualem parameters in tabulated form for the given soil name SOILNS (example in Table 10).

Table 10 Example of the Van Genuchten-Mualem database file.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>* Database of parameters for the Van Genuchten-Mualem models of</td>
<td></td>
</tr>
<tr>
<td>* TBNAM</td>
<td>name of soil</td>
</tr>
<tr>
<td>* TKS</td>
<td>saturated hydraulic conductivity ( K_s ) (cm ( d^{-1} ))</td>
</tr>
<tr>
<td>* TND</td>
<td>( n ) parameter (drying curve)</td>
</tr>
</tbody>
</table>
* TL
  \( \lambda \) parameter
* TALP
  \( \alpha \) parameter (cm\(^{-1}\))
* TALPD
  \( \alpha_p \) parameter (cm\(^{-1}\))
* TALPW
  \( \alpha_w \) parameter (cm\(^{-1}\))
* TWCS
  saturated volumetric water content \( \theta_s \) (-)
* TWCR
  residual volumetric water content \( \theta_r \) (-)

\begin{align*}
\text{TBNAM} & & \text{TKS} & & \text{TND} & & \text{TL} & & \text{TALP} & & \text{TALPD} & & \text{TALPW} & & \text{TWCS} & & \text{TWCR} \\
\hline
\text{HEINEN}, & & 1997. \text{PhD Thesis WAU (cm/d); a coarse sand} & & \text{median .6 mm).} \\
's488t' & & 1256.0 & & 4.98171 & & 0.52581 & & 0.06069 & & 0.06069 & & 0.11745 & & 0.326 & & 0.01573 \\
's488b' & & 1256.0 & & 4.90919 & & 0.52581 & & 0.05312 & & 0.05312 & & 0.09466 & & 0.311 & & 0.02311 \\
\text{OPPEN}, & & 1994. \text{PhD Thesis WAU (cm/d); a peat (75\%) - perlite (25\%) mixture.} & & \text{wilfred'} & & 8640.0 & & 1.42 & & 2.35 & & 0.13 & & 0.13 & & 0.90 & & 0.92 & & 0.0 \\
\text{DA SILVA ET AL,} & & 1995. \text{Acta Hortic. 401:71-75. (cm/d).} & & \text{rockwool'} & & 6192. & & 3.90471 & & -0.28288 & & 0.0873 & & 0.0873 & & 0.55363 & & 0.92402 & & 0.00673 \\
\text{* some others (cm,d)} & & & & & & & & & & & & & & & & & & \\
\text{rubicalm'} & & 25.92 & & 3.301 & & 0.5 & & 0.0136 & & 0.0136 & & 0.0378 & & 0.381 & & 0.17 \\
\text{'guelphl'} & & 31.68 & & 2.14 & & 0.5 & & 0.0098 & & 0.0098 & & 0.0196 & & 0.434 & & 0.219 \\
\text{'glendale'} & & 13.1 & & 1.3954 & & 0.5 & & 0.0104 & & 0.0104 & & 0.0208 & & 0.4686 & & 0.106 \\
\text{'berino'} & & 541.0 & & 2.239 & & 0.5 & & 0.028 & & 0.028 & & 0.056 & & 0.3658 & & 0.0286 \\
\end{align*}

IS
With the variable IS = 1 (see example 6.2), it is possible to consider exponentially (both in x and z directions) distributed root water uptake (default: IS = 0). In that case the following additional parameters should be supplied.

<table>
<thead>
<tr>
<th>TRANSP</th>
<th>transpiration rate (cm ( \text{d}^3 ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>extinction coefficient in x direction (cm(^{-1}))</td>
</tr>
<tr>
<td>Q</td>
<td>extinction coefficient in z direction (cm(^{-1}))</td>
</tr>
</tbody>
</table>

Table 11 Example input file SOIL.DAT.

* data file for program FUSSIM2 containing soil parameters: dimensions, * soil physical parameters, and if desired plant root uptake parameters * for spatially distributed exponential root water uptake *
* descriptive title of the case studied TITLE = 'Test run, sandbl'

* Number of columns NC and layers NL
NC = 10
NL = 26

* inside codes: first NC values refer to row 1, etc.
INSIDE = 260*1

* thickness of soil columns DX and thickness of soil layers DZ
DX = 10*10.0
DZ = 16*5.0, 10*2.0

* how to treat conductivity CTREAT
* CTREAT = 0 : compute according to Van Genuchten function
* CTREAT = 1 : compute according to Gardner function
* CTREAT = 2 : conductivity and capacity are constant
* then supply CONWON (cm/d) and CONCAP (1/cm)

CTREAT = 0

* soil physical properties of the soil
* NSOILS : number of different soil types
* FILNAM : (+)name of database file where properties are stored
* SOILS : NSOILS names of soil types (which are present in FILNAM)
* ISOIL : for each control volume a soil code must be given; first NC * values for first layer, then NC values for second layer, etc.

NSOILS = 1
* KS in FILNAM must be cm/d; program converts units corresponding to
* UNITS as supplied in timer file
FILNAM = 'c:\user\soils\SOILS.DBF'
SOILNS = 'zandbl'
ISOIL = 260*1

* KWAY determines how to average K at the faces of the control volumes
  * KWAY < 0 arithmetic average
  * KWAY = 0 geometric average
  * KWAY > 0 harmonic average

KWAY = 0

* parameter determining whether spatially distributed exponential root
* water uptake is to be considered (IS <> 0) or not (IS = 0)
* If IS = 1 then supply values for P(1/cm), Q(1/cm) and TRANSP (cm/d)
IS = 0

---

5.3.4 Input file BOUNDS.DAT

This file contains the (time independent) boundary conditions, internal conditions, and initial h distribution (example in Table 12). Time variable boundary conditions, in this case rain or irrigation and evapotranspiration data, are given in the file WNAME.

NSEEPE

The variable NSEEPE contains the number of seepage faces present in the flow domain (≤ 5). For each of the seepage faces the column (ISEEP?) and row (JSEEPEP?) numbers should be supplied (with a maximum of 20 nodes per seepage face). The ? must refer to a seepage face number. For example, if two seepage faces are considered, the user must supply: NSEEPE = 2, and data for the arrays ISEEPEP1, JSEEPEP1, and ISEEPEP2, JSEEPEP2.

Table 12 Example input file BOUNDS.DAT.

* data file for program FUSSIM2 containing boundary, internal and initial
* conditions
* ITOPE: pointer to boundary condition at top
  * ITOPE < 0 : prescribed pressure head (HTOP) at top boundary
  * ITOPE = 0 : no flux across top boundary
  * ITOPE = 1 : flux equal to input by rain and/or irrigation only
  * ITOPE = 2 : flux equal to output due to evaporation only
  * ITOPE = 3 : flux equal to difference in input and output (default)

ITOP = 10*3
HTOP = 10*0.0

* IBOT: pointer to boundary condition at bottom
  * IBOT < 0 : prescribed pressure head (HBTOP) at lower boundary
  * IBOT = 0 : seepage drainage at lower boundary (old option, now define
    Seepage face with NSEEPE etc.)
  * IBOT = 1 : prescribed flux (FBOT) at lower boundary (default)
  * IBOT = 2 : free drainage or unit hydraulic gradient
  * IBOT = 3 : resistance drain at lower boundary (supply H0 and DRRES)

IBOT = 10*1

* constant pressure head at bottom; only of importance if IBOT < 0
HBTOP = 10*0.0

* known flux at bottom; only of importance if IBOT = 0 (cm/d)
* program converts units corresponding to UNITS as supplied in timer file
FBOT = 10*0.0

* left boundary conditions
* ILEFT: pointer to boundary condition at left boundary
  * ILEFT < 0 : prescribed pressure head (HLEFT) at left boundary
  * ILEFT = 0 : no flow at left boundary
  * ILEFT > 0 : prescribed flux (FLEFT) at left boundary

ILEFT = 25*1,-1
HLEFT = 26*0.0
FLEFT = 26*0.0
right boundary conditions
  * IRIGHT: pointer to boundary condition at right boundary
  * IRIGHT < 0: prescribed pressure head (IRIGHT) at right boundary
  * IRIGHT = 0: no flow at right boundary
  * IRIGHT > 0: prescribed flux (FRIGHT) at right boundary
IRIGHT = 10*1, 16*1
HRIGHT = 10*0.0, 2.5, 7.5, 12.5, 17.5, 22.5, 27.5, 31., 33., 35., 37.,
  39., 41., 43., 45., 47., 50.
FRIGHT = 26*0.0

* internal conditions
  * INTRN: pointer to boundary condition at internal node
  * INTRN < 0: prescribed pressure head (HINTRN) at internal node
  * INTRN > 0: prescribed flux (FINTRN) at internal node
HINTRN = 260*0
HINTRN = 260*0.0
FINTRN = 260*0.0

* initial h distribution for flow domain
  * first NC values for first layer, second NC values for second layer etc.
  * if only 1 value is supplied, this means that the soil profile is in
  * equilibrium with this pressure head pertaining to the bottom; no
  * horizontal gradients exist
HINI =
-100.0 -92.5 -87.5 -82.5 -77.5 -72.5 -67.5 -62.5 -57.5 -50.0
-92.5 -85.0 -80.0 -75.0 -70.0 -65.0 -60.0 -55.0 -50.0 -45.0
-82.5 -75.0 -70.0 -65.0 -60.0 -55.0 -50.0 -45.0 -40.0 -35.0
-77.5 -70.0 -65.0 -60.0 -55.0 -50.0 -45.0 -40.0 -35.0 -30.0
-72.5 -65.0 -60.0 -55.0 -50.0 -45.0 -40.0 -35.0 -30.0 -25.0
-67.5 -60.0 -55.0 -50.0 -45.0 -40.0 -35.0 -30.0 -25.0 -20.0
-62.5 -55.0 -50.0 -45.0 -40.0 -35.0 -30.0 -25.0 -20.0 -15.0
-57.5 -50.0 -45.0 -40.0 -35.0 -30.0 -25.0 -20.0 -15.0 -10.0
-52.5 -45.0 -40.0 -35.0 -30.0 -25.0 -20.0 -15.0 -10.0 -5.0
-47.5 -40.0 -35.0 -30.0 -25.0 -20.0 -15.0 -10.0 -5.0  0.0
-42.5 -35.0 -30.0 -25.0 -20.0 -15.0 -10.0 -5.0  0.0  5.0
-37.5 -32.5 -25.0 -20.0 -15.0 -10.0 -5.0  0.0  5.0 10.0
-27.5 -20.0 -15.0 -10.0 -5.0  0.0  5.0 10.0 15.0 20.0
-22.5 -15.0 -10.0 -5.0  0.0  5.0 10.0 15.0 20.0 25.0
-19.0 -11.5 -6.5 -1.5  3.5  8.5 13.5 18.5 23.5 28.5
-17.0 -9.5 -4.5  5.5 10.5 15.5 20.5 25.5 30.5 35.5
-15.0 -7.5 -2.5  2.5  7.5 12.5 17.5 22.5 27.5 32.5
-13.0 -5.5 -0.5  4.5  9.5 14.5 19.5 24.5 29.5 34.5
-11.0 -3.5  1.5  6.5 11.5 16.5 21.5 26.5 31.5 36.5
-9.0 -1.5  3.5  8.5 13.5 18.5 23.5 28.5 33.5 38.5
-7.0  0.5  5.5 10.5 15.5 20.5 25.5 30.5 35.5 40.5
-5.0  2.5  7.5 12.5 17.5 22.5 27.5 32.5 37.5 42.5
-3.0  4.5  9.5 14.5 19.5 24.5 29.5 34.5 39.5 44.5
  0.0  7.5 12.5 17.5 22.5 27.5 32.5 37.5 42.5 50.0

* number of seepage faces
NSEEFP = 1
JSEEFP = 20*1
JSEEFP = 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21,
  22, 23, 24, 25

5.3.5 Input file TIMER.DAT

Data file containing general variables controlling computations of FUSSIM2 (example in Table 13). These are timer data, such as initial time step, end time of simulation, print times, and control data for the solution procedure, such as convergence criteria and hysteresis control data.

UNITS
The program assumes that all length units are in cm. With respect to time, the user supplies the time units UNITS, either as d (days), h (hours), m (minutes) or s (seconds). The program requires that all variables given by the user, which have time in their dimensions, are supplied with dimension d. The program automatically converts these dimensions to the user supplied UNITS.
There is one exception to this rule. The time-dependent variables RAIN, TPOT, EPOT and IRRINT (all in file WNAME) MUST be given in time units UNITS.

**CONPRI, PRDEL, PRTIME**

Printing times at constant interval: CONPRI = 1, interval is PRDEL. Printing at user supplied times: CONPRI = 0, print times (< 400) given in array PRTIME.

**MAXIT**

The maximum number of iterations to obtain convergence. In case the ICCG procedure is used, the number of iterations used in ICCG is 10*MAXIT.

**ISOLVE**

The variable ISOLVE indicates which solution procedure is to be used.

- **ISOLVE = 0**  ICCG method
- **ISOLVE = 1**  ADI method, use Eqs. [116]-[121] when unsaturated, use Eqs. [122]-[127] when (partly) saturated; change between the two methods at pressure head HSAT as defined in file FUS2.CTR
- **ISOLVE = 2**  ADI method, use Eqs. [116]-[121] all the times (when partly saturated conditions occur, the program generally crashes)
- **ISOLVE = 3**  ADI method, use Eqs. [122]-[127] (large mass balance errors can be expected)
- **ISOLVE = 4**  use ADI (as in ISOLVE = 2) when flow domain is completely unsaturated while during partly saturated conditions use ICCG (as in ISOLVE = 0); the change between the two methods occurs near saturation at a pressure head HSAT, as given in file FUS2.CTR. This option is not thoroughly tested.

**OUTYES**

The variable OUTYES determines what kind of output is desired. Output in tabulated form. There is always some default output each printing time, such as mass balance information, and total flow across the boundaries.

---

**Table 13  Example input file TIMER.DAT.**

* datafile for program FUSSIM2 containing time control data and iterations
* stop criterion

```plaintext
<table>
<thead>
<tr>
<th>UNITS</th>
<th>'d'</th>
<th>time units, e.g., d, h, min, s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>! NOTE THAT all input variables in which time</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! appears in the units should be given with</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! time as days</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! program converts units corresponding to</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! UNITS as supplied in timer file</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! this counts for:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! KSAT, FBOT, FLEFT, FRIGHT, FINTRN</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! CONCON, TRANSP, DRRES</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! K1, LRVK, LRVT, LRVTS (module TRANSP)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! FMAX, PLUPT, DIF0 (module SOLUTE)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>! NOTE THAT : RAIN, TPOT, EPOT and IRRINT</td>
</tr>
</tbody>
</table>
```

* timer variables below must be in UNITS !!!

```plaintext
| DELT | 1.0E-5 | time step |
| DTMAX | 2.5E-1 | maximum allowable time step |
| CONDEL | 0 | constant time step: 1: yes, else no |
| ZBTA | 0.01 | maximum allowable change in water content |
| CONPRI | 1 | constant print time step: 1: yes, else no |
| PRDEL | 1.0 | ! print interval for results (if CONPRI = 1) |
| PRTIME | 0.0, 10.0, 15.0, 20.0, 300.0 | ! end time of simulation |
| FINTIM | 300.0 | ! iterations stop criterion, e.g. 1.0E-4 |
| EPSIL | 1.0E-04 | ! iterations stop criterion for ICCG method |
| EPSILII | 1.0E-08 | ! e.g. 1.0E-8 |
| MAXIT | 20 | ! maximum number of iterations |
|       |     | ! the ICCG solution procedure uses |
```
5.3.6 Input file WEATHER.DAT

The time-dependent (top) boundary conditions are given in file WNAME (example in Table 14). The information present depends on the choice of the variable METHIR in file FUS2.CTR (see description over there). As mentioned in the description of file TNAMES, the time units for the variables in the file WNAME MUST be equal to that defined in the variable UNITS in file TNAMES.

Table 14 Example input file WEATHER.DAT.

<table>
<thead>
<tr>
<th>*</th>
<th>Supply the following information depending on the value of METHIR:</th>
</tr>
</thead>
<tbody>
<tr>
<td>* METHIR = 0</td>
<td>RAIN, TPOT, EPOT</td>
</tr>
<tr>
<td>* METHIR = 1</td>
<td>TPOT, EPOT, IRRINT, LFRAC, ETPH</td>
</tr>
<tr>
<td>* METHIR = 2</td>
<td>TPOT, EPOT, IRRINT, LFRAC, HTRESH, JTRESH</td>
</tr>
<tr>
<td>* METHIR = 3</td>
<td>TPOT, EPOT, IRRINT, LFRAC, ECRESH, ITRESH, JTRESH</td>
</tr>
</tbody>
</table>

* All variables must be in cm/UNITS, with UNITS defined in file TNAMES.
* rain or irrigation (RAIN), potential evaporation (EPOT) and potential transpiration (TPOT)

RAIN = 300*1.0
EPOT = 300*0.0
TPOT = 300*0.0

5.3.7 Input file TRANSP.DAT

Input data for the root water uptake module are given in the file TRANSP (example in Table 15).

REDPOT
Yes (REDPOT = 1) or not (REDPOT = 0) use the transpiration reduction function Eqs. [25] and [26],
i.e. if REDPOT = 0 force always potential transpiration.

RTGROW
Yes (RTGROW = 1) or not (RTGROW = 0) consider logistic root growth. If not, the variable LRVINI contains the constant root length density distribution. If logistic root growth is considered, the variable LRVINI contains the maximum (asymptotic) root length density values. Additionally, the user should supply the following data.

- LRVK: the inverse time constant (d³)
- LRVT: the time of inflection of the logistic curve (d)
- LRVT5: start time of simulation relative to start of plant growth, i.e. the age of the roots at start of simulation (d)

The logistic growth equation is (Heinen, 1997; TIME is the current simulation time)

\[
LRV = \frac{LRVINI}{1 + e^{-LRVK(TIME - LRVT - LRVT5)}}
\]

Table 15  Example input file TRANSP.DAT.

* solute reflection coefficient (-)
SIGMA = 0.9

* osmotic pressure head inside plant (cm)
HOSP = 0.

* root conductance K1 (cm/d)
* program converts units corresponding to UNITS as supplied in timer file
K1 = 3.6D-06

* root radius R0 (cm)
R0 = 0.017

* reduction parameter REDPOT; if REDPOT > 0 then reduction
* of transpiration
REDPOT = 1

* using Campbell reduction function with two parameters: A and HRHALF
A = 10.0
HRHALF = 1.0D4

* reference pressure head for determination of matric flux potential
* point out which variables have to be printed
OUTTRA = 0,

  0,  ! print root water uptake rate (cm/UNITS) and cumulative
   0,  ! Root water uptake since start (cm): 1: yes, else no
   0,  ! print root water uptake rate per cm root length
   0,  ! (cm)/cm root.UNITS): idem
   1,  ! print relative contribution of root water uptake in
   1,  ! relation to actual transpiration rate (-): idem
   0,  ! print root pressure head (cm): idem
   1,  ! print actual transpiration rate (cm/UNITS): idem
   1,  ! print realized root water uptake (cm/UNITS), which
   ! should be equal to actual transpiration rate: idem

* consider logistic root growth (RTGROW = 1) or not (RTGROW = 0; default)
RTGROW = 0

* constant (RTGROW = 0) or maximum (RTGROW = 1) distribution of root
* length density in control volumes;
* first NC values for first layer, then NC values for second layer, etc.
LRVINI =
3*3.4927,
3*3.4927,
3*3.4927,
3*2.4400,
3*2.4400,
3*2.4400,
3*0.7983,
3*0.7983,
3*0.7983,
3*0.

* growth rate parameter, i.e. k of logistic model (1/d): LRVK
* time of inflection, i.e. t* of logistic model (d): LRVT
* start time of simulation, i.e. time to be added to simulation
* time in order to get real time (d): LRVT
* program converts units corresponding to UNITS as supplied in timer file
LRVK  = 2.157D-1
LRVT  = 21.0D0
LRVTS = 13.0D0

5.3.8 Input file TRANSP.CTR

In the file TRANSP.CTR some control parameters are given used in the root water uptake module (example in Table 16).

TRANS
The variable TRANS indicates what kind of root water uptake model is to be used. By default the root water uptake model of Section 2.3 is used. As an alternative, root water uptake may also be considered as water uptake from a control volume proportional to root length in that control volume Eq. [113] (e.g. under wet conditions).

TRHYST
Do not change this parameter.

Table 16 Example input file TRANSP.CTR.

| TRANS   | 'COMPUTE'       | 'COMPUTE' : use water uptake model (default) |
| FAC     | 5.0             | 'PROPORT' : root water uptake proportional to root length |
| RDPMIN  | 1.0E-4          | increase/reduction factor for finding proper minimum and maximum values for root pressure head |
| NP      | 3               | convergence criterion root water uptake |
| TOL     | 1.0E-4          | number of points used for interpolation in matric flux potential table |
| TRHYST  | 'N'             | accuracy used for root finding procedure |
|         |                 | Yes or No use hysteretic approximation in TRANS |

5.3.9 Input file TGEN.DAT

The file TGEN.DAT contains some parameters used by the root water uptake module (example in Table 17). The matric flux potential needed in the root water uptake model (Section 2.3) is not at all times computed, due to the large computation time. Instead, initially a table is constructed from which the matric flux potential is obtained through linear interpolation. The number of entries in the table is NNTAB, the smallest pressure head for which the table is to be constructed is PPBIG, the largest pressure head is PPEND, and the reference pressure head is PPREF (PPREF > PPBIG). Note that the absolute values of pressure head need to be given. The range [PPEND,PPBIG] must include all pressure heads that can be expected to occur during simulation. For very coarse porous media, it may be difficult to obtain the matric flux potential table when PPBIG and PPREF are very large; then, use smaller values for these variables.

Table 17 Example input file TGEN.DAT.
5.3.10 Input file SOLUTE.DAT

The input data for solute transport are given in file SNAME (example in Table 18). Additional information for the several ions to be considered are read from file IONSINFO.DAT (see below). It is assumed that the boundary conditions (JTOP, JBOT, JLEFT, JRIGHT) apply equally to all ions present in solution (see IONSINFO.DAT). However, for each ion present the concentration at boundary must be supplied (CTOP, CBOT, CLEFT, CRIGHT). For example, if only two ions, e.g. N and P are used, CTOP contains 2 times NC data: first NC values for N and second NC values for P (data for ions not present must not be supplied).

FREQF
The variable FREQF can be used in some special cases. For example, if fertigation is controlled by a threshold EC value (METHIR = 3, see file FUS2.CTR) the variable FREQF determines the frequency of nutrient solution that is applied, while at the other times only pure water is applied.

IDISP
The variable IDISP determines which dispersivity model is used. If IDISP = 0, then a single dispersivity LD is to be supplied (Eq. [172] is used), while if IDISP = 1 (default) the longitudinal and transversal dispersivities AL and AT should be supplied (Eqs. [161]-[163] are used).

ICON
The initial distribution can be given as initial concentration (CONC: mmol l⁻¹) (ICON > 0), or as initial amount (AMOUNT) per control volume (ICON ≤ 0). For ICON = 0 AMOUNT is given in mmol, for ICON < 0 AMOUNT is given in mg. Computations are always done in mmol; output is always in mmol.

Table 18 Example input file SOLUTE.DAT.

* top boundary
  * JTOP = -1 : fixed concentration CTOP
  * = 0 : no flow of solutes across boundary
  * = +1 : prescribed flux density: water flux density times a) CTOP
  * (when flow into domain), or b) CONC (when outflow occurs)
  JTOP = 10*0
  CTOP = 10*0.

* bottom boundary
  * JBOT = -1 : fixed concentration CBOT
  * = 0 : no flow of solutes across boundary
  * = +1 : prescribed flux density: water flux density times a) CBOT
  * (when flow into domain), or b) CONC (when outflow occurs)
  JBOT = 10*0
  CBOT = 10*0.

* left boundary
  * JLEFT = -1 : fixed concentration CLEFT
  * = 0 : no flow of solutes across boundary
  * = +1 : prescribed flux density: water flux density times a) CLEFT
  * (when flow into domain), or b) CONC (when outflow occurs)
  JLEFT = 10*0, 16*1
  CLEFT = 26*0.

* right boundary
  * JRIGHT = -1 : fixed concentration CRIGHT
  * = 0 : no flow of solutes across boundary
  * = +1 : prescribed flux density: water flux density times a)
* CRIGHT (inflow), or b) CONC (outflow)
JRIGHT = 26*1
CRIGHT = 26*0.1

* frequency of using nutrient solution every irrigation event
* FREQP = 3 means use nutrient solution every third irrigation event
FREQP = 1

* IDISP : method of dispersivities
*    IDISP = 0 \quad \text{use single dispersivity \text{LD}}
*    IDISP = 1 \quad \text{use longitudinal and transversal dispersivities \text{AL} and \text{AT}} \quad \text{(Default)}
IDISP = 1

* dispersion length (cm)
LD = 10.0

* longitudinal and transversal dispersivities \text{AL} and \text{AT}
AL = 2.0
AT = 0.2

* three parameters describing two linear parts of the impedance
* \text{(FIMP) water content relationship}
* \text{CP1: slope, CP2: intercept, WCLOW: water content where two linear relationships intersect}
CP1 = 260*1.58 \quad \text{! sand or loam (clay: 0.99)}
CP2 = 260*-0.17 \quad \text{! sand, loam, or clay}
WCLOW = 260*0.12 \quad \text{! sand or loam (clay: 0.20)}

* parameter ICON determines whether the following table contains initial
* \text{CONcentration (ICON > 0) or AMOUNT (ICON <= 0) data}
ICON = 1

* initial concentration distribution; first NC values for layer 1, then
* NC values for layer 2, etc. (mmol/1) (ICON>0)
* in case AMOUNT is given: mmol (ICON=0) or mg/cm (ICON<0)
CONC = 260*5.0

* what to print
OUTSLT = 1, \quad \text{! yes (1) or no (0) write concentration}
0, \quad \text{! yes (1) or no (0) write amount}
1, \quad \text{! yes (1) or no (0) write salt fluxes in x-dir.}
1, \quad \text{! yes (1) or no (0) write salt fluxes in z dir.}
0, \quad \text{! yes (1) or no (0) write uptake rate}
0, \quad \text{! yes (1) or no (0) write cumulative uptake}
0, \quad \text{! yes (1) or no (0) write EC}

---

5.3.11 Input file IONSINFO.DAT

General information about the ions possibly present in solution is given in the file IONSINFO.DAT (example in Table 19).

Table 19 Example input file IONSINFO.DAT.

* Information of 13 individual ions, needed for EC computations in module
* SOLUTE
IONNAM name of ion (for output)
IONYES yes (1) or not (0) consider ion in computations
VALENC valence of ion
MOBIL ionic mobility (cm2/(s.V))
IONRAD diameter of ion (supply in Angstroms, 1 Angstrom = 10^-10 m)
DIFG diffusion of ion in free water (cm2/d)

IONYES = 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
IONNAM = \{'NO3', 'K', 'H2PO4', 'Ca', 'Mg', 'PO4', 'Cl', 'Na', 'NH4', 'HCO3', 'CO3', 'H', 'OH'
VALENC = 1, 1, 1, 2, 2, 2, 1, 1, 1, 2, 1, 1
* MOBIL must be in units [cm²/(s.V)] (not using time units d, h, m !!!)
MOBIL = 7.41E-4, 7.62E-4, 7.84E-4, 6.17E-4, 5.50E-4, 8.29E-4, 7.91E-4,
5.19E-4, 7.62E-4, 4.61E-4, 7.46E-4, 3.63E-3, 2.01E-3

* Ångstrom !!!

* cm²/d
* program converts units corresponding to UNITS as supplied in timer file
DIF0 = 1.64, 1.69, 1.74, 0.685, 0.610, 0.920, 1.76,
     1.15, 1.69, 1.02, 0.828, 8.06, 4.46

* To compute ion activity coefficient, three equations can be used:
* DEBYE = 0 extended Debye-Hückel (default),
* DEBYE = 1 approximation for dilute solutions,
* DEBYE = 2 approximation for concentrated solutions
* DEBYE = 3 use approximations for dilute and/or concentrated
* solutions

* Of course, approximation are only used when applicable, i.e. a dilute
* solution has ionic strength I < 0.005, and a concentrated solution has
* ionic strength I > 0.1; if not, the standard Debye-Hückel theory will
* always be used
DEBYE = 0

* Parameters A and B can be computed or can be constant; if constant,
* they should be given
* PARAB = 0 constant, then give PARA (mol^0.5/kg^0.5) and PARB
*     (mol^0.5/(kg^0.5 m))
*     = 1 compute (not available, since temperature is not
*     computed)
PARAB = 0
PARA = 0.51 ! mol^0.5/kg^0.5
PARB = 0.33 ! mol^0.5/(kg^0.5 m); the actual value is 0.33.10^10,
! but the power 10^10 is left out, since IONRAD is given
! in Ångstrom (10^-10)

5.3.12 Input file UPTA.DAT

Data file for root solute uptake are given in the file UPTA.DAT (example in Table 20).

IUPWAY
When the root nutrient uptake model of section 2.6 is to be used the variable IUPWAY = 1 (default).
As an alternative root nutrient uptake proportional to root length can be considered by setting
IUPWAY = 0.

METHOD
Root nutrient uptake according to the model presented in Section 2.6 is represented by METHOD >
0. If METHOD = 0, the mass flow component in the model is not considered, i.e. only diffusion to
the root is considered. As a special case, METHOD < 0, the model presented in Section 2.6 is used
with now mass flow computed as water uptake times concentration.

NPLANT, PLUPT
The required uptake per plant (PLUPT) is multiplied by the total number of plants (NPLANT) in the
flow domain to get the required uptake from the flow domain.

Table 20 Example input file UPTA.DAT.

* which uptake routine to use
5.4 Examples of output files

A simulation run results in one or two user-supplied output files (RNAME and SNAME, see Section 5.3), a logfile (FUS2.LOG), and several intermediate files not important to the user. Of these intermediate files the 'TMP' are deleted from the current directory when simulation is finished properly, and files with extension 'TAB' remain on the current directory. The latter files can be safely deleted by the user. The file FUS2.LOG contains some messages from the TUTIL reading routines, which are of no importance to the user. If supplied by the user it can contain all the time steps that were used by the model.

The water results are written to the user-supplied output file RNAME (example in Table 21); solute results are printed to the user-supplied file SNAME (example in Table 22). Examples of these two files are given below, and should be self-explanatory.

Table 21 Example of water results file RNAME.

<table>
<thead>
<tr>
<th>Example 5.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Units of measure:</td>
</tr>
<tr>
<td>Length in : cm (default).</td>
</tr>
<tr>
<td>Time in : d (user supplied).</td>
</tr>
<tr>
<td>Output filename : c-w</td>
</tr>
<tr>
<td>Soil conditions file name : c-so</td>
</tr>
<tr>
<td>Boundary and initial conditions filename : c-bc</td>
</tr>
<tr>
<td>Weather conditions filename : c-wn</td>
</tr>
<tr>
<td>Timer data filename : c-tm</td>
</tr>
<tr>
<td>GEOMETRY</td>
</tr>
<tr>
<td>Profile width (cm) : 200.00</td>
</tr>
<tr>
<td>Profile depth (cm) : 200.00</td>
</tr>
<tr>
<td>Number of grid points in x : 20</td>
</tr>
</tbody>
</table>
Number of grid points in z : 24

Position gridpoints
X-coordinate gridpoints (cm)
0.00 15.00 25.00 35.00 45.00 55.00 65.00 75.00 85.00 95.00 105.00 115.00 125.00
135.00 145.00 155.00 165.00 175.00 185.00 200.00
Thickness control-volumes in x (cm)
10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00
10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00
Z-coordinates gridpoints (cm)
0.00 15.00 25.00 35.00 45.00 55.00 65.00 75.00 85.00 91.00 93.00 95.00 97.00
99.00 105.00 115.00 125.00 135.00 145.00 155.00 165.00 175.00 185.00 200.00
Thickness control-volumes in z (cm)
10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 2.00 2.00 2.00 2.00
2.00 2.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00

Scheme of flow domain nodes with coded boundary conditions.
R : rain or irrigation input only
E : evaporation only
N : R - E
h : prescribed pressure head
f : known flow across boundary
- : f = 0
s : seepage face
x : two boundary conditions
u : unit gradient or free drainage
d : seepage drain
r : resistance drain

Soil type codes:

Code  Name
-----------------------------------------------
1  zavelb7

xNx
xNx11-
XNx111-
Xx11111-
Xx111111-
sNNNNNN11111111-
sl1llllllllllllll-
sl1llllllllllllll-
sl1llllllllllllll-
sllllllllllllll-
sllllllllllllll-
sl1llllllllllll-
sllllllllllll-
sl1llllllllll-
sllllllllll-
sl1lllllll-
slllllll-
sl1lllll-
slllll-
sl1lll-
slll-
sll-
sl-
s-
x-------------------

TIMER VARIABLES
DELT : 1.00000E-05 d
PRDEL : 1.00000E+00 d
FINTIM : 1.00000E+01 d

Variable time step with:
DTMAX : 2.50000E-01 d
ZETA : 1.00000E-02 d

Convergence based on minimal change in H and K.
Maximum number of iterations = 20
Convergence criterion EPSIL = 1.00000E-04
Convergence criterion EPSIL = 1.00000E-08

Hydraulic properties for each of the control volumes.
van Genuchten functions used.
| 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 |
| 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 |

**Net total flow into flow domain:**
4.000000000E+02 ml/d

**Total amount that passed top layer:**
4.000000000E+00 ml

**Total amount that passed bottom layer:**
0.000000000E+00 ml

**Total amount that passed left boundary:**
1.72900011065E+19 ml

**Total amount that passed right boundary:**
0.000000000E+00 ml

**TIME = 1.000000000E+01**

**Total water:**
1.5964142542E+04 ml

**Total change water:**
4.0595609950E+02 ml

**Relative water:**
1.00000070567E+01 ml

**Water content [-]:**
4.00000E+00, 4.00000E+01, 4.00000E+01, 4.00000E+01, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00

**Pressure head (cm):**
4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00

**Relative head [cm]:**
4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00, 4.00000E+00
Net total flow into flow domain: 1.2351368758E-02 m³/d
Total amount that passed top boundary: 2.7563260082E+03 ml
Total amount that passed bottom layer: 0.0000000000E+00 ml
Total amount that passed left boundary: -2.3504010148E+03 ml
Total amount that passed right boundary: 0.0000000000E+00 ml

Table 22: Example of solute results file SNAME.

<table>
<thead>
<tr>
<th>TIME</th>
<th>0.00000000E+00</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total nutrient</td>
<td>1.2078535348E+10 mmol</td>
</tr>
<tr>
<td>Total change nutrient</td>
<td>0.0000000000E+00 mmol</td>
</tr>
<tr>
<td>Total uptake nutrient</td>
<td>0.0000000000E+00 mmol</td>
</tr>
<tr>
<td>Balance nutrient</td>
<td>-2.6649659458E-13 mmol</td>
</tr>
<tr>
<td>Relative nutrient</td>
<td>-2.7060731895E-15</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Initial</th>
<th>0.000000E+00</th>
<th>0.000000E+00</th>
<th>0.000000E+00</th>
<th>0.000000E+00</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td></td>
<td>1.000000E-01</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
</tr>
<tr>
<td></td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
</tr>
</tbody>
</table>
1. Total amount of N that passed top layer = -6.9777991507E+00 mmol
2. Total amount of N that passed bottom layer = 0.0000000000E+00 mmol
3. Total amount of N that passed left boundary = 0.0000000000E+00 mmol
4. Total amount of N that passed right boundary = 0.0000000000E+00 mmol

TIME = 1.0000000000E+01
5.5 The rerun facility

There is a special utility in the TTUTLIB library (Rappoldt & Van Kraanling, 1990) which makes it
possible to make reruns. For each run one or more variables can be changed. Reruns are carried out when in the current directory a file named RERUNS.DAT is present. In this file the new data for one or more variables (as appearing in any of the files discussed in Section 5.3) are given. It is required that for each run the same variables are used and in the same order. An example of a rerun file is given in Table 23. Note that the first run is described by the individual files, while the following runs use the same initial data, except for the new data given in the RERUNS.DAT file.

Table 23  Example of a RERUNS.DAT file.

* run 2
soilns = 'zandb1'
rain = 365*1.0
wname = 'zand2'
* run 3
soilns = 'zandb1'
rain = 365*1.5
wname = 'zand3'
* run 4
soilns = 'kleib10'
rain = 365*0.5
wname = 'klei1'
* run 5
soilns = 'kleib10'
rain = 365*1.0
wname = 'klei2'
* run 6
soilns = 'kleib10'
rain = 365*1.5
wname = 'klei3'

In this example six runs are done, three with a soil named ‘zandb1’ and three with a soil named ‘kleib10’. For the two soils three rain regimes are considered: either 0.5, 1.0 or 1.5 cm/d precipitation. For each case a separate output file is used.

A RERUN.LOG file is produced in the current directory in which the adapted values are given, or where explanations for possible errors are given.

5.6 Computer requirements

The simulation model FUSSIM2 is programmed in Fortran 77, and compiled with Microsoft Fortran 32 v. 1.0 visual workbench. In this way extended memory can be used. The user must have available some files belonging to this compiler, i.e. mmd.396 and dosxnt.386. These files should be referred to in the Windows SYSTEM.INI file under the header [386Enh] as follows:

[386Enh]
device=<path>\mmd.386
device=<path>\dosxnt.386

Moreover, some Microsoft Fortran facilities have been used to enhance screen output. This works properly when in the CONFIG.SYS file the following statement is given:

DEVICEHIGH=<path>\ANSI.SYS

Example runs in Chapter 6 were carried out on a Compaq Deskpro with an Intell Pentium 166 MHz processor. The model has been used also on a Alpha mainframe computer, using a locally available Fortran compiler.
6 Some examples

In this chapter we present some example simulations with the model described in this report. The first example is carried out to verify the correctness of the solution procedure ADI or ICCG, by comparing the change in time of pressure head with a transient, analytical solution. The second example compares the steady state distribution of pressure head with an exponentially distributed (both in x and z directions) sink term with an analytical solution for this problem. The third example presents a comparison between simulated and analytical results for transient solute transport with or without uniform water flow. The fourth example shows the results of simulations carried out for a sand bed system. The fifth example shows the results for an irregular flow domain. The sixth example is given to indicate the effect of the osmotic pressure head for root water uptake in a sand bed system. Input data for all examples are listed in Appendix 3.

6.1 Linear, transient flow in an unsaturated rectangular flow domain

Case 1
Carlaw & Jaeger (1959, p. 173, Eqs. 11 and 6) gave an analytical solution for the temperature distribution in a finite rectangle (-X/2 < x < X/2, -Z/2 < z < Z/2) as a function of time with unit initial temperature and zero temperature at the surface. It is given as a product

\[ u = \psi \left( \frac{x}{2} \right) \psi \left( \frac{z}{2} \right), \tag{204} \]

where the function \( \psi \) is defined as

\[ \psi (\sigma, \tau) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \exp \left( -\frac{k (2n+1)^2 \pi^2 \tau}{4 \tau^2} \right) \cos \left( \frac{(2n+1) \pi \sigma}{2 \tau} \right). \tag{205} \]

In Eq. [204] \( u \) represents a scaled temperature. In our case it can be seen as a reduced pressure head defined as where \( h_r \) equals the pressure head at the boundary, and \( h_i \) the initial internal pressure head. The constant \( k \) in Eq. [205] is analogous to the diffusivity \( D_w \), which is defined as (Koo revaar et al., 1983)

\[ D_w = \frac{K}{C} \tag{206} \]

Note that \( D_w \) in this case is constant. The solution of Eq. [204] for given time \( t \) and \( D_w \) can be computed, and comparison with numerical solutions can be done. The program FUSSIM2 was ran with the ratio \( K/C \) constant and equal to \( D_w \). That is, both \( K \) and \( C \) were kept constant at the value 1.0. Moreover, the influence of gravity was neglected. Instead of starting with physical initial pressure heads, reduced pressure heads were used: zero at the boundary and one inside the flow domain. A square flow domain was used, with \( X = Z = 10.0 \) cm.

Results and discussion of case 1
Note that due to symmetry we need to consider only a quarter of the flow domain. The analytical and simulated results are presented in Fig. 9. As time progresses the distribution of \( u \) flattens, it tends to the final steady state situation where \( u \) becomes zero everywhere in the flow domain. The simulated results closely describe the analytical solution. As a measure for the deviation between the simulated and analytical solution (Table 24) we define
Simulated (markers) and analytical (solid lines) reduced pressure heads $u$ as a function of horizontal distance $x$ for the linear transient flow case with uniform initial $u$ distribution (case 1): (A) for time $t = 1$ d, and (B) for time $t = 10$ d. In each graph the top data refer to the vertical positions $z = 0.6$ cm and the bottom data refer to $z = 5$ cm.

$$\delta = \sum_{i=1}^{n} \left( \frac{\text{num}_i - \text{an}_i}{\text{an}_i} \right)^2,$$

where $\text{num}$ represents the numerical value at a certain position, $\text{an}$ the corresponding analytical value, and $n$ is the total number of nodes. The deviations between the analytical and numerical solutions are due to the fact that at the boundaries of the flow domain the initial gradient of $u$ is infinitely large. This cannot be numerically simulated. Better results are obtained by increasing the number of grid lines. There are, however, other cases where the initial gradient of $u$ is finite, as is demonstrated in case 2. The use of iterations appeared to be necessary. Although the problem is linear, use of the simulation model without iterations yielded erroneous results, especially near the boundaries.
Table 24  Run time of the model (on a Compaq prolinea 590), relative mass balance error, and the deviation $\delta$ between the simulated and analytical solutions according to Eq. [208] for two times, for the three solution procedures present in the model: ICCG (Section 3.3.2), ADI using Eqs. [116]-[121] (ADI, 1) or ADI using Eqs. [122]-[127] (ADI, 2) (Section 3.3.1).

<table>
<thead>
<tr>
<th>Procedure</th>
<th>Run time (s)</th>
<th>Relative mass balance error $(t = 10 \text{ d})$</th>
<th>$\delta (t = 1 \text{ d})$</th>
<th>$\delta (t = 10 \text{ d})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICCG</td>
<td>36.0</td>
<td>$-9.3 , 10^7$</td>
<td>2.83 $10^4$</td>
<td>2.25 $10^2$</td>
</tr>
<tr>
<td>ADI, 1</td>
<td>17.4</td>
<td>$-2.9 , 10^5$</td>
<td>2.83 $10^4$</td>
<td>2.26 $10^2$</td>
</tr>
<tr>
<td>ADI, 2</td>
<td>17.4</td>
<td>$-4.8 , 10^5$</td>
<td>2.88 $10^4$</td>
<td>1.47 $10^3$</td>
</tr>
</tbody>
</table>

Case 2
In this case the initial reduced pressure head, $u$, is zero at the boundaries and parabolic inside the flow domain, such that at the boundary the gradient of $u$ is finite. The analytical solution is given by Carslaw & Jaeger (1959, p. 98, Eq. 16), again as a product analogous to Eq. [204]

$$u = \phi\left(x, \frac{X}{2}\right) \phi\left(z, \frac{Z}{2}\right), \quad [208]$$

with the function $\phi$ defined as

$$\phi\left(\sigma, \tau\right) = \frac{32 \, V_o}{\pi^3} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^3} \exp\left(-k \frac{(2n+1)^2 \pi^2 t}{4 \tau^2}\right) \cos\left(\frac{(2n+1) \pi \sigma}{2 \tau}\right). \quad [209]$$

The parameters are the same as in case study 1. the constant $V_o$ is defined in the initial condition function, $u_i$

$$u_i = V_o \left(\frac{X}{2}\right)^2 - \left(\frac{X}{2}\right)^2 \left(\frac{Z}{2}\right)^2$$

$$u_i = V_o \left(\frac{X}{2}\right)^2 - \left(\frac{Z}{2}\right)^2$$

$$\left(\frac{X}{2}\right)^2 - \left(\frac{Z}{2}\right)^2$$

[210]

Since the flow is linear the initial condition is a product of initial parabolic functions in $x$ and $z$ direction. $V_o$ represents the maximum value of the parabolic initial condition in both the $x$ and $z$ direction, i.e. $V_o^2$ is the maximum occurring at $(x,z) = (X/2,Z/2)$. In this case study we used $V_o = D_w = K = C = 1.0$, and $X = Z = 10.0 \text{ cm}$.

Results and discussion of case 2
The analytical and simulated results are presented in Fig. 10, and the corresponding differences between numerical and analytical solutions, $\delta$, according to Eq. [208] are presented in Table 25. The deviations $\delta$ are somewhat larger for the larger time step simulations.
Figure 10  Simulated (markers) and analytical (solid lines) reduced pressure heads $u$ as a function of horizontal distance $x$ for the linear transient flow case with parabolic initial $u$ distribution (dotted lines) (case 2): (A) for time $t = 1$ d, and (B) for time $t = 10$ d. In each graph the top data refer to the vertical positions $z = 0.6$ cm and the bottom data refer to $z = 5$ cm.

Table 25  Run time of the model (on a Compaq prolinea 590), relative mass balance error, and the deviation $\delta$ between the simulated and analytical solutions according to Eq. [208] for two times, for the three solution procedures present in the model: ICCG (Section 3.3.2), ADI using Eqs. [116]-[121] (ADI, 1) or ADI using Eqs. [122]-[127] (ADI, 2) (Section 3.3.1). With ADI, 2 two runs were carried out, first with $c = 10^{-8}$ and second with $c = 10^{-8}$.

<table>
<thead>
<tr>
<th>Procedure</th>
<th>Run time (s)</th>
<th>Relative mass balance error</th>
<th>$\delta (t = 1$ d)</th>
<th>$\delta (t = 10$ d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICCG</td>
<td>22.9</td>
<td>$-5.6 \times 10^{-3}$</td>
<td>$1.32 \times 10^{-3}$</td>
<td>$3.99 \times 10^{-1}$</td>
</tr>
<tr>
<td>ADI, 1</td>
<td>10.2</td>
<td>$-4.0 \times 10^{-5}$</td>
<td>$1.32 \times 10^{-3}$</td>
<td>$4.00 \times 10^{-1}$</td>
</tr>
<tr>
<td>ADI, 2; $c = 10^{-4}$</td>
<td>10.2</td>
<td>$-9.4 \times 10^{-3}$</td>
<td>$3.28 \times 10^{-4}$</td>
<td>$2.35 \times 10^{-1}$</td>
</tr>
<tr>
<td>ADI, 2; $c = 10^{-6}$</td>
<td>32.3</td>
<td>$2.3 \times 10^{-4}$</td>
<td>$1.31 \times 10^{-3}$</td>
<td>$3.97 \times 10^{-1}$</td>
</tr>
</tbody>
</table>
6.2 Two-dimensional, non-linear, steady-state flow in unsaturated soil with explicitly known root water uptake

The governing flow equation for water for steady state flow in a rectangular flow domain with a spatially distributed sink strength can be written as

\[
\frac{\partial}{\partial x} (K \frac{\partial h}{\partial x}) + \frac{\partial}{\partial z} (K \frac{\partial h}{\partial z}) - \frac{\partial K}{\partial z} - A^*(x,z) = 0.
\]  

[211]

The source/sink term \( S_w \) in Eq. [4] is here given as \( A^*(x,z) (A^* > 0) \), which is explicitly known and a function of space only. It is preceded by a minus sign to represent a sink. The left, right and upper boundaries are considered as no-flow boundaries, and the bottom boundary is considered as a prescribed pressure head boundary. It is assumed that \( K \) depends on \( h \) by the following exponential relationship (Gardner, 1958)

\[
K(h) = K_0 e^{\alpha h}.
\]  

[212]

where \( \alpha \) (L\(^{-1}\)) is known as the sorptive number of the soil and is a measure of capillary properties of the soil. It is different from the \( \alpha \) parameter in the Van Genuchten-Mualem model as described in Chapter 4. In general, soils with strong capillary effects tend to have a small value of \( \alpha \), e.g. 0.002 cm\(^{-1}\) or less, and coarse soils tend to have a large value of \( \alpha \), e.g. 0.2 cm\(^{-1}\) or more (Philip, 1989). The value 2\( \alpha^2 \) is known as the sorptive length of the soil (Philip, 1989). The value \( \alpha^2 \) can be interpreted as a characteristic length of the soil (Raats & Gardner, 1971). Now with Eq. [213] Eq. [212] can be transformed to

\[
\frac{\partial^2 K}{\partial x^2} + \frac{\alpha^2 K}{\partial z^2} - \alpha \frac{\partial K}{\partial z} - 2 \alpha A^*(x,z) = 0.
\]  

[213]

Due to this transformation Eq. [214] now is a linear partial differential equation. The boundary conditions, as described below Eq. [212], are now given as

\[
\frac{\partial K}{\partial x} = 0, \quad x = 0, \quad x = X,
\]  

[214]

\[
\frac{\partial K}{\partial x} = K_0, \quad z = 0,
\]  

[215]

and

\[
K = K_0, \quad z = Z.
\]  

[216]

It is assumed that the sink term is given by

\[
A^*(x,z) = A_0^* e^{-px} e^{-qz},
\]  

[217]

where \( p \) and \( q \) are extinction coefficients (L\(^{-1}\)) in the \( x \) and \( z \) directions, respectively. Raats (1974) used the one-dimensional form of Eq. [218]. The sink term can be regarded as root water uptake, where the root density exponentially decreases in the \( x \) and \( z \) directions (all parts of the root take up water at the same rate). The constant \( A_0^* \) in Eq. [218] can be evaluated by considering that the integral of \( A^* \) over the total domain should be equal to the transpiration rate \( T \) (L T\(^{-1}\)) times the profile width \( X \) according to

\[
\int_0^X \int_0^z e^{-px} e^{-qz} dx \, dz = X T.
\]  

[218]
Solving Eq. [219] yields

$$A_0^* = \frac{pqXT}{(1 - e^{-px})(1 - e^{-qz})}.$$  \hspace{1cm} [219]

In Appendix 4 a full derivation of the complete solution is presented. Here we give only the solution itself. The solution gives the hydraulic conductivity expressed in dimensionless variables as

$$K(\zeta, \xi) = \frac{B_1 + B_2 e^{-\lambda \zeta} + A_0 \phi(0)}{b (b + \lambda)} + 2 \sum_{n=1}^{\infty} \left( B_3 e^{m_s \xi} + B_4 e^{m_s \xi} \right) \cos(n \xi)$$

$$- 2 A_0 e^{b \xi} \sum_{n=1}^{\infty} \frac{\phi(n)}{n^2 - \beta^2} \cos(n \xi),$$  \hspace{1cm} [220]

with

$$B_1 = \pi K = \frac{A_0 \phi(0)}{b (b + \lambda)} + \frac{A_0 \phi(0)}{b \lambda} e^{b \zeta},$$  \hspace{1cm} [221]

$$B_2 = - \frac{A_0 \phi(0) e^{b \zeta}}{b \lambda},$$  \hspace{1cm} [222]

$$B_3 = \frac{A_0 \phi(n)}{n^2 - b (b + \lambda)} \frac{e^{b \zeta} (b + \lambda) - e^{m_s \xi} (m_2 + \lambda)}{e^{m_s \xi} (m_1 + \lambda) - e^{m_s \xi} (m_2 + \lambda)},$$  \hspace{1cm} [223]

and

$$B_4 = - \frac{A_0 \phi(n)}{n^2 - b (b + \lambda)} \frac{e^{b \zeta} (b + \lambda) - e^{m_s \xi} (m_1 + \lambda)}{e^{m_s \xi} (m_1 + \lambda) - e^{m_s \xi} (m_2 + \lambda)}.$$  \hspace{1cm} [224]

The dimensionless variables \( \zeta \) and \( \xi \) are given as

$$\zeta = \frac{\pi}{X} (Z - z),$$  \hspace{1cm} [225]

and

$$\xi = \frac{\pi}{X} (X - x).$$  \hspace{1cm} [226]

The remaining dimensionless variables \( \zeta, A_0, \lambda, a, b \) and \( \beta \), and the variables \( m_1, m_2 \) and \( \phi(n) \) occurring in Eqs. [221]-[225] are defined in Appendix 4.

In the numerical model FUSSIM2 the constant root water uptake per time step at node \((i,j)\) is obtained by integrating Eq. [218] over the control volume as follows
\[ A^\ast(I,J) = \int_{x_{i+1}}^{x_i} \int_{z_{i+1}}^{z_i} A_0^* e^{px} e^{-qz} dx \, dz , \]  

[227]

yielding

\[ A^\ast(I,J) = \frac{A_0^*}{p \, q} \left( e^{-p \Delta x_i} - 1 \right) \left( e^{-q \Delta z_i} - 1 \right). \]

[228]

Since this sink term is constant it can be subtracted from the 'knowns' parameter \( b \) given in Eq. [76], i.e.

\[ b(I,J) = b(I,J) - A^\ast(I,J). \]

[229]

Simulations were carried out for a rectangular soil profile of depth \( Z = 75 \) cm and of width \( X = 30 \) cm. The following parameters were used: \( \alpha = 0.05 \) cm\(^{-1} \), \( K = 20 \) cm day\(^{-1} \), \( p = 0.3 \) cm\(^{2} \) day\(^{-1} \), \( q = 0.046 \) cm\(^{-1} \), and \( T = 0.5 \) cm day\(^{-1} \). The steady state \( h \) distribution over \( x \) at three depths is presented in Fig. 11A. The top of the profile is drier near \( x = 0 \) than at \( x = X \). Deeper in the profile the \( h \) distribution becomes more or less horizontal. Compared to the equilibrium situation, when \( h \) at \( z = 0.0, 8.33 \) and \( 50.0 \) cm would be constant at \(-75.0, -66.67 \) and \(-25.0 \) cm, respectively, the whole soil profile is drier due to root water uptake. Note that the \( h \) distributions intersect the lines \( x = 0 \) and \( x = X \) perpendicularly, which is a consequence of the chosen no-flow boundary conditions here. In Fig. 11B the \( h \) distribution over \( z \) is presented for three positions of \( x \), together with the equilibrium

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure11}
\caption{Simulated (markers) and analytical (solid lines) pressure head \( h \) distributions for two-dimensional, non-linear, steady-state flow in unsaturated soil with explicitly known plant root water uptake: (A) \( h \) as a function of horizontal distance \( x \) for three depths \( z \), and (B) \( h(z) \) for three positions of \( x \). The equilibrium \( h(z) \) condition when no sinks are present is denoted by the dotted line.}
\end{figure}
situation. Closer to the upper left corner, where root water uptake is largest, the soil has dried the most. Deeper in the soil profile the soil is slightly drier than the equilibrium situation, since root water uptake decreases exponentially with $z$. Note that the slopes $dh/dz$ of the analytical solutions at $z = 0$ approach 1, a consequence of the no-flow boundary condition at the top of the soil profile. In general, the numerical results describe the analytical results well.

6.3 Transient solute transport under steady-state water conditions

In this section we will compare analytical solutions for solute transport under steady-state water conditions with simulation results. It can be regarded as verification of the solute transport module of FUSSIM2. We will consider two one-dimensional cases: diffusive transport and dispersive-diffusive transport in a column. In this example no sources or sinks are considered.

Case 1
Consider a soil column of length $X$. There is no water movement in the column so that $\theta$, $q_x$, and $q_z$ are constant, i.e. $\theta = 0.4$ and $q_x = q_z = 0$. Solute transport occurs in one dimension, and Eq. (32) with Eq. [33] now is written as

$$\theta \frac{\partial c}{\partial t} = \theta D_0 \frac{\partial}{\partial x} \left( \frac{\partial c}{\partial x} \right).$$

For $\theta = 0.4$, $\theta D_0 \tau(\theta)$ for NO$_3$ is constant and equal to 0.303072 cm$^2$/d$^2$. Equation [231] is analogous to the heat transport equation for linear flow in slab with constant heat conductivity. For the case when a no-flow condition is present at $x = 0$ and when at $x = X$ a constant concentration $c_r$ is maintained, the solution of Eq. [231], for uniform initial concentration $c_o$, is given as (Carslaw & Jaeger, 1959, based on their Eq. (5) on p. 101)

$$c(x,t) = c_r +$$
$$+ \frac{2}{X} \sum_{n=0} \exp\left\{ -D_0 \tau(\theta) \left( \frac{(2n+1) \pi}{2X} \right)^2 t \right\} \cos\left( \frac{(2n+1) \pi x}{2X} \right) \left( \frac{2X}{(2n+1) \pi} \right) (-1)^n (c_o - c_r).$$

Results case 1
There is a good resemblance between the analytical and simulated $c(x,t)$ results for times $t = 10$ d and $t = 50$ d (Fig. 12), especially when taking into account that at $t = 0$ the gradient, and thus the solute flux density, at $x = X$ is infinitely large (see also discussion case 1 in Section 6.1). The deviations according to Eq. [208] at $t = 10$ d and $t = 50$ d: $\delta = 9.3 \times 10^{-2}$ and $\delta = 1.7 \times 10^{-2}$, respectively.

Case 2
For the classical case of one-dimensional convective-diffusive transport we use the solution of Lapidus & Amundsen (1952; see also Van Genuchten & Alves, 1982). Consider an infinitely long soil column with a constant initial concentration $c_o$ with a constant boundary concentration $c_r$, condition at $x = 0$, and with no concentration gradient condition at $x = \infty$. As for the first case mentioned in this section, we consider uniform water (flow) conditions. The governing transport equation is given as

$$\theta \frac{\partial c}{\partial t} = (a_x q_x + \theta D_0 \tau(\theta)) \frac{\partial^2 c}{\partial x^2} - q_x \frac{\partial c}{\partial x}.$$

For $\theta = 0.4$, $q_x = 0.1$ cm$^2$/d$^2$ and $q_z = 2.0$ cm, $a_x q_x + \theta D_0 \tau(\theta)$ for NO$_3$ is constant and equal to 0.503072 cm$^2$/d$^2$. The solution $c(x,t)$ can be given as
Figure 12
Simulated (markers) and analytical (lines) concentration $c$ profiles as a function of horizontal distance $x$ with uniform initial $c$ distribution for two times $t = 10$ and $50$ d for the diffusion only case (case 1).

Figure 13
Simulated (markers) and analytical (lines) concentration $c$ profiles as a function of horizontal distance $x$ with uniform initial $c$ distribution for four times $t = 5, 10, 25$ and $50$ d for the convection plus diffusion case (case 2).
where \( v = q_y / \theta \) and \( D = (a.q_x + \theta D_c \epsilon (\theta)) / \theta \).

**Results case 2**

For several times we obtain a good comparison between simulated and analytical \( c(x,t) \) profiles (Fig. 13). The deviations according to Eq. [208] at \( t = 5, 10, 25 \) and \( 50 \) d are \( \delta = 1.2 \times 10^{-3}, 5.8 \times 10^{-3}, 1.1 \times 10^{-3}, \) and \( 7.2 \times 10^{-3} \), respectively.

In general, the explicit numerical solution of the solute transport equation is reliable. It is verified by comparing it to two analytically available solutions.

### 6.4 Water flow and solute transport in a sand bed system

Heinen (1997) used the model to describe the dynamics of water and solutes in a coarse sand bed system. The sand bed system is schematically presented in Fig. 14, and the boundary conditions for water movement are indicated. The boundary conditions for solute transport are, except at the dripper location at the top and at the seepage drain at the bottom, all of no-flow type. At the dripper location a nutrient solution enters the flow domain, with the solute flux density given as the irrigation rate times the concentration of the nutrient solution. At the seepage drain at the bottom solutes can leave the sand bed when drainage occurs; the solute flux density then given as the drainage rate times the local concentration. In this case hysteresis was an important feature to

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**Figure 14** Schematic representation of half the region between two drains of the sand bed system showing the boundary conditions for water movement (from Heinen, 1997).
account for. All further details can be found in the thesis of Heinen (1997). The simulation model was well able to describe measured volumetric water content profiles (Fig. 15), measured pressure head profiles, and measured cumulative drainage outflow. When hysteresis was not taken into account much too wet conditions were predicted and thus no agreement between simulated and measured data were obtained.

A laboratory breakthrough experiment in two dimensions, using a small sand bed system, was carried out to determine the dispersivities $a_y$ and $a_z$ (Fig. 16). Then it was possible to simulate the dynamics of nitrogen in the sand bed system. At the upper left corner of the sand bed system increased concentrations developed (Fig. 17). During fertigation only a short period of time this region is diluted with the fresh incoming solution. Drainage soon starts after the beginning of fertigation, resulting in a direct movement of incoming solution from the dripper towards the drain, so that the upper left corner is not refreshed.

With the help of this simulation model alternative fertigation strategies can be developed in order to obtain a more uniform salt profile in the root zone.

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Figure 15 Simulated (lines) and measured (markers) volumetric water content $\theta$ as a function of time $t$ in half the region between two drains of the sand bed system at three depths $z$, with (solid lines) and without (dotted lines) regarding hysteresis (after Heinen, 1997).
Figure 16  Breakthrough curve measured (markers) in a small sand bed system with drip application and predicted (lines) by the simulation model for the indicated values of the longitudinal \( a_L \) and transversal \( a_T \) dispersivities. The x-axis represents the volume \( V_s \) of solution applied relative to the volume \( V_f \) of solution present in the sand bed, and the y-axis represents the concentration \( c \) of the effluent relative to the influent concentration \( c_f \) (from Heinen, 1997).

Figure 17  Simulated N concentration \( c \) (mmol l\(^{-1}\)) distribution in half the region between two drains of the sand bed system: (A) before the start of a fertigation period, and (B) just before the end of fertigation (160 minutes later) (from Heinen, 1997).
6.5 Example with an irregular flow domain, a ditch and a seepage face

The model has been used for an irregular flow domain by De Willigen et al. (1995), who simulated water flow and nitrogen transport in a potato ridge, and by Heinen (1997) who simulated water flow and nitrogen transport in a rockwool slab with a planting cube. Here we give results for some arbitrary flow domain where a ditch with constant water level is present, and in which the wall of the ditch above the water level is regarded as a seepage face. Thus water movement from the soil towards the ditch may occur through the wetted boundary, or by seepage through the boundary above the water level. The soil surface has a slope, which is simulated by a stepwise upper boundary.

A near steady-state situation is reached at $t = 10$ d. The water flux densities computed across each CV interface were used to compute a net flux density for the centers of each CV. With the help of the graphical software package XY (Van Heerden & Tikta, 1994) water movement is visualized in Fig. 18. Water movement in the unsaturated zone is primarily vertical, except near the ditch. In the saturated zone there is a dominant horizontal component of water flow. Water flows radially towards the ditch. The ground water level lies above the constant water level in the ditch, due to incoming rain at the top of the soil profile. Seepage at the dry ditch wall occurs along a length of 2 cm.

The output file contains integrated amounts of water and solute that passed the four boundaries separately. If we consider only the ditch, we can obtain the amounts that left the flow domain into the ditch. For this purpose, the amount that passed the top layer was diminished with the amount of rain input across the interval $x = 30$ cm to $x = 200$ cm. After $t = 2$ d a near steady state outflow of water occurs, but not for the solute (Fig. 19). The amount of solute that enters the ditch becomes less in time, since the total storage decreases in time; there is no addition of solute in the flow domain. Up to time $t = 4$ d the outflow through the bottom of the ditch has a concentration of 0.01 mmol ml$^{-1}$, i.e. 10 mmol l$^{-1}$ which is the initial concentration of the soil profile, meaning that up to day 4 the concentration at the bottom of the soil profile was still at the initial level.

![Figure 18](image)

Simulated water flux density distribution in the example with irregular boundaries and a ditch with a seepage face. The size of the arrows represents the relative magnitude of the water flux density. The shaded area represents the saturated zone.
The amount of water (solid markers) and solute (open markers) that entered the ditch as a function of time $t$. The total amount is split into contributions that entered the ditch through the side wall and through the bottom.

### 6.6 Effect of osmotic potential on root water uptake

In Eq. [20] the osmotic potential in the root water uptake description was introduced. De Willigen & Heinen (1998) investigated the effect is of the osmotic potential on root water uptake for the sand bed system of Heinzen (1997; see also example 6.4). For details, the reader is referred to De Willigen & Heinen (1998). Here we give some of their findings. First, the interaction between distribution of roots and distribution of salts was investigated using Eq. [20]. According to the calculations it is not so much the average concentration which has much significance, but the distribution of concentration with respect to that of the root distribution. When $L_{p}$ decreases exponentially with depth, the case with the salts also decreasing exponentially with depth resulted in the highest value for $h$. When the salt distribution increased with depth the smallest value for $h$ was obtained. An intermediate value for $h$ was obtained when a uniform salt distribution was assumed. Simulation runs were carried out for conditions when no effect of osmotic potential was considered ($\sigma = 0$), or when the effect of osmotic potential was most pronounced (worst case with $\sigma = 1$ and $h_{p} = 0$). Simulations pertained to the sand bed system which was allowed to dry out for 12 days. Total water uptake was compared to potential total water uptake. As a reference case realistic values for $h_{p}$ and $c_{s}$ were used. In case osmotic potential is taken into account, halving the value of $h_{p}$ did not have much effect on actual water uptake, but doubling $c_{s}$ did have a pronounced effect (Fig. 20). The effect of excluding or including the osmotic potential can be seen in the EC distribution (Fig. 21) and in the water uptake distribution (Fig. 22) in the sand bed system. The distribution in case of $\sigma = 0$ (no effects of osmotic head; top diagram in Fig. 21) is much more pronounced: the solutes accumulating in the upper 5 cm. In case of $\sigma = 1$ (bottom diagram in Fig. 21) the increase in concentration at the substrate surface near the plant positions is much smaller. This difference is due to the distribution of the cumulative water uptake as given in Fig. 22. In case of osmotic head effects the water has been taken up from deeper layers, in fact in the upper layers water has been transported from the roots into the soil, thereby diluting the soil solution. This outflow of water from the roots is a consequence of the way the water uptake is described, and could be an artefact. Outflow of water from roots, however, has been experimentally observed (e.g. Baker & Van Bavel, 1986).
Figure 20  Cumulative uptake of water by the root system for three combinations of parameter $h_{r,1/2}$ and initial concentration $c_i$ compared to the potential demand (from De Willigen & Heinen, 1998). Results refer to the sand bed system presented in Fig. 14.

The main conclusion (see Fig. 20) by De Willigen & Heinen (1998) was that under normal conditions as found in Dutch horticulture, osmotic effects on water uptake are not important, but that this depends on the distribution of salts with respect to that of the roots. On the other hand, it may explain typical EC distributions in the root zone.
Figure 21  Electrical conductivity EC distributions in the sand bed system after the twelve-day simulation period with $h_{w2} \approx 4750$ cm and twice the normal initial concentration for the cases without ($\sigma = 0$, top diagram) and with ($\sigma = 1$, top diagram) inclusion of osmotic head in water uptake equation (Eq. [20]) (from De Willigen & Heinen, 1998).

Figure 22  Cumulative water uptake distributions in the sand bed system after the twelve-day simulation period corresponding to the cases of Fig. 21. A negative uptake means outflow of water from the roots, see text for explanation (from De Willigen & Heinen, 1998).
References


Appendix 1  On the computation of $\phi$

The computation of $\phi$ in Eq. [7], with $K(h)$ given by Mualem’s (1976) expression Eq. [187] is not directly possible, since the integral $\int K(h)dh$ is unknown. The solution can be obtained by using a numerical integration method, e.g. the Romberg integration routine of Press et al. (1986). For computational simplicity reasons a transformed expression for $K(h)$ is used. The new integration variable $h'$ is defined as

$$h' = \ln |\alpha h|.$$  \[A1-1\]

Thus

$$dh = \frac{e^{h'}}{\alpha} dh'.$$  \[A1-2\]

Then $\phi$ is obtained from

$$\phi = \frac{K_s}{\alpha} \int_{h_1}^{h_2} \left[ \frac{(1 + e^{nh'})^m - e^{(n-1)h'}}{(1 + e^{nh'})^m(h')} \right]^2 e^{nh'} dh'.$$  \[A1-3\]

In order to avoid large computational times in evaluating $\phi$ in the root water uptake module, use is made of tabulated $\phi(h)$ obtained once before the start of simulation. In the simulation model $\phi$ is obtained by linear interpolation.
Appendix 2  On the Function $P$

The definition of the function $P$ in the text follows from Mualem (1984) from whom we quote:

"... The independent domain theory assumes that all pore domains are free to drain independently, though in reality pores can drain only when free access to outside air is formed. Thus, the pore domain ability to drain is rather dependent on the state of the surrounding pores. To account for this phenomenon, a domain dependence factor ($P_d$) is applied. Following Everett (1975) and Mualem & Dagan (1975), $P_d$ is considered to be a macroscopic variable that depends on the actual $\theta$. By definition, $P_d$ describes the relative portion of the drainable pores...".

Mualem (1984) defined $P_d$ as follows

$$P_d = \frac{\Delta \theta}{\Delta \theta_0},$$  \hspace{1cm} \text{[A2-1]}

where $\Delta \theta$ represents the change in $\theta$ of the latest drying process that has occurred, and $\Delta \theta_0$ represents the change in $\theta$ corresponding to the identical process, but in the absence of blockage of air access - namely, $P_d = 1$, as if the pore water domains were actually independent. Mualem (1984) then gives the domain dependence factor in explicit form, using the main drying characteristic and main wetting characteristic. This is given as Eq. [191] in the text.

Some special attention is given here to evaluating the function $P$, defined in Eq. [191] of the main text, in case of the scanning drying curve. The water content for which Eq. [189] of the main text is valid is found iteratively using Brent's method (Press et al., 1986; function ZBRENT described in their chapter 9.3). Although the derivative of Eq. [189] of the main text is known, i.e. Eqs. [195]-[199] of the main text, and thus a fast Newton-Raphson method could be used as well, this is not done because of the complexity of the derivative expression. Brent's method finds the root of the function

$$f(\theta) = \theta(h) - \theta_d + P(\theta)[\theta_s - \theta_w(h) + \theta_w(h_a) - \theta_w(h)],$$  \hspace{1cm} \text{[A2-2]}

for which $f(\theta) = 0$. The accuracy at which $x$ is to be obtained is given as $\epsilon_\theta$, i.e. $\epsilon_\theta = 10^{-4}$. The range where $x$ is to be found is obviously $[\theta_s, \theta_d]$. Unfortunately, Brent's method fails at the boundary values, so that a somewhat smaller initial guess of the range is used as input: $[\theta_s + \epsilon_i, \theta_s + \epsilon_i]$, with $\epsilon_i$ set to a small number, i.e. $\epsilon_i = 10^{-4}$. However, the length of the range can be decreased, since we know the last reversal point and a scanning drying curve is followed. The new range than becomes $[\theta_s + \epsilon_i, \theta_s + \epsilon_i]$, with $\epsilon_i$ set to some value because of safety reasons, i.e. $\epsilon_i = 0.01$. These new boundaries may not exceed the maximum boundaries $\theta_s + \epsilon_i$ or $\theta_s - \epsilon_i$. An example of the function $f(\theta)$ for a fictive soil with $\theta_d = 0.2$ cm$^3$ cm$^{-3}$ and $h_a = -54.1$ cm is given in Fig. A2-1. It is obvious that there is only one root for which $f(\theta) = 0$, and thus ZBRENT's module will yield a unique estimate for $\theta$. Since the scanning drying curve is followed, $|h| > |h_a|$, and thus the curve for $h = -10$ in Fig. A2-1 is meaningless. For a very large pressure head, e.g. $h = -1000$ cm in Fig. A2-1, the function $f(\theta)$ is always larger than zero, and no value for $\theta$ will be obtained, and thus ZBRENT's method will fail.

Presumably, this situation never occurs, and the scanning drying curve will have crossed the main drying curve and the function $f(\theta)$ needs not to be evaluated anymore. Moreover, it is still possible that the true new water content value searched for is in the range $[\theta_d, \theta_s + \epsilon_i]$ or $[\theta_s - \epsilon_i, \theta_s]$. In that case nothing happens, i.e. $\theta^{new} = \theta^i$. When the status $\kappa_n$ of a node changes to 1 or $+1$, some constants in Eqs. [189] and [190], respectively, are computed. For the node under consideration the constants $\theta_d$ and $\theta_w(h_a)$ occurring in Eq. [189] (when $\kappa_n = -1$) are computed and stored, while for Eq. [190] (when $\kappa_n = +1$) the constants $\theta_d$, $\theta_w(h_a)$ and $P(\theta_s)(\theta_s - \theta_w(h_a))$ are computed and stored.
$f(\theta)$ as defined in Eq. [A2-2] (-)

Figure A2-1  Example of function $f(\theta)$ (Eq. [A2-2]) for a fictive soil with $\theta_s = 0.2$ (-) and $h_s = -54.1$ cm.
Appendix 3  Summary of input data for examples of chapter 6

Input data used in example of Section 6.1.

Case 1
(1a) ICCG solution procedure
(1b) ADI solution procedure using Eqs. [116]-[121]
(1c) ADI solution procedure using Eqs. [122]-[127]

Case 2
(2a) ICCG solution procedure
(2b) ADI solution procedure using Eqs. [116]-[121]
(2c) ADI solution procedure using Eqs. [122]-[127], \( \epsilon_c = 10^4 \)
(2d) ADI solution procedure using Eqs. [122]-[127], \( \epsilon_c = 10^8 \)

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<td>0.2241562</td>
</tr>
<tr>
<td>0.6820071</td>
<td>0.7646745</td>
</tr>
<tr>
<td>0.9681638</td>
<td>0.987241</td>
</tr>
<tr>
<td>0.0</td>
<td>0.2256</td>
</tr>
<tr>
<td>0.6864</td>
<td>0.7696</td>
</tr>
<tr>
<td>0.9744</td>
<td>0.9936</td>
</tr>
</tbody>
</table>

Weather data n.a.

Timer control data

$\Delta t_p, \Delta t_{max}, \Delta t_{min}, t_p, \zeta, m_t$ $10^{-5}, 0.25, 10^{-5}, 10.0, 0.01, 1.5$

Solution procedure

procedure (1a,2a) ICCG, (1b,2b) ADI using Eqs. [116]-[121], (1c,2c,2d) ADI using Eqs. [122]-[127]

$\epsilon$, max. # iterations (1a,1b,1c,2a,2b,2c) $10^{-4}$ (2d) $10^{-6}$, 20

ICCG: $\epsilon$, max. # iterations (1a,2a) $10^{-8}$, 200

Hysteresis n.a.

Solute transport n.a.

Root data n.a.

Root water uptake n.a.

Root nutrient uptake n.a.
<table>
<thead>
<tr>
<th>Irrigation control unit</th>
<th>n.a.</th>
</tr>
</thead>
</table>

n.a. = not applicable
Input data used in example of Section 6.2.

<table>
<thead>
<tr>
<th>Basic units</th>
<th>cm, d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow domain configuration</td>
<td></td>
</tr>
<tr>
<td>$N, M$</td>
<td>16, 31</td>
</tr>
<tr>
<td>$\Delta x_j$ (N values)</td>
<td>1.0, 14*2.0, 1.0</td>
</tr>
<tr>
<td>$\Delta z_j$ (M values)</td>
<td>1.25, 29*2.5, 1.25</td>
</tr>
<tr>
<td>substrate</td>
<td>hypothetical soil: $\theta_i = 0$, $\theta_s = 0.4$, $n = 1.1$; Gardner (1958) exponential $K(h)$ relationship with $K_i = 20$ cm d$^{-1}$ and $\alpha = 0.05$ cm$^{-1}$</td>
</tr>
<tr>
<td>top boundary condition: $q_{\text{top}}, h_{\text{top}}$ (N values)</td>
<td>$q_{\text{top}}$: 16*0.0</td>
</tr>
<tr>
<td>top boundary condition: $q_{\text{bottom}}, h_{\text{bottom}}$ (N values)</td>
<td>$h_{\text{bottom}}$: 16*0.0</td>
</tr>
<tr>
<td>left boundary condition: $q_{\text{left}}, h_{\text{left}}$ (M values)</td>
<td>$q_{\text{left}}$: 31*0.0</td>
</tr>
<tr>
<td>right boundary condition: $q_{\text{right}}, h_{\text{right}}$ (M values)</td>
<td>$q_{\text{right}}$: 31*0.0</td>
</tr>
<tr>
<td>$h_0$ (MxN values, or equilibrium)</td>
<td>equilibrium with $h = 0$ cm at the bottom</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Weather data</th>
<th>n.a.</th>
</tr>
</thead>
<tbody>
<tr>
<td>irrigation rate</td>
<td>n.a.</td>
</tr>
<tr>
<td>$T_p$</td>
<td>analytical root water uptake with TRANSP = 0.5 cm d$^{-1}$, $P = 0.3$ cm$^{-1}$, $Q = 0.046$ cm$^{-1}$</td>
</tr>
<tr>
<td>$E_p$</td>
<td>n.a.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Timer control data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t, \Delta t_{\text{max}}, \Delta t_{\text{min}}, t_j, \zeta, m_t$</td>
<td>$10^5$, 0.25, $10^{-5}$, 40.0, 0.01, 1.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Solution procedure</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>procedure</td>
<td>ICCG, ADI (both types)</td>
</tr>
<tr>
<td>$e_{\text{crit}}$, max. # iterations</td>
<td>$10^4$, 20</td>
</tr>
<tr>
<td>ICCG: $e_{\text{crit}}$, max. # iterations</td>
<td>$10^8$, 200</td>
</tr>
</tbody>
</table>

| Hysteresis           | n.a.        |
| Solute transport     | n.a.        |
| Root data            | n.a.        |
| Root water uptake    | n.a. (See under $T_p$ and text for explanation) |
| Root nutrient uptake | n.a.        |
| Irrigation control unit | n.a. |

n.a. = not applicable
Input data used in example of Section 6.3.
(a) Case 1
(b) Case 2

| Basic units | cm, d |
| Flow domain configuration | |
| $N, M$ | (a) 20, 5; (b) 30, 5 |
| $\Delta x_i$ (N values) | (a) 20*10.0; (b) 4*0.25, 2*0.5, 3*1.0, 2*2.5, 19*5.0 |
| $\Delta z_i$ (M values) | 5*2.0 |
| substrate | zavelb7 from the 'Staringreeks' (Wösten et al., 1994) |
| top boundary condition: $q_{top}$, $h_{top}$ (N values) | no flow (steady state situation defined in THHFXFZ.DAT) |
| bottom boundary condition: $q_{bottom}$, $h_{bottom}$ (N values) | no flow (steady state situation defined in THHFXFZ.DAT) |
| left boundary condition: $q_{left}$, $h_{left}$ (M values) | (a) no flow (steady state situation defined in THHFXFZ.DAT) |
| | (b) uniform horizontal flow $q_x = 0.1$ (steady state situation defined in THHFXFZ.DAT) |
| right boundary condition: $q_{right}$, $h_{right}$ (M values) | (a) no flow (steady state situation defined in THHFXFZ.DAT) |
| | (b) uniform horizontal flow $q_x = 0.1$ (steady state situation defined in THHFXFZ.DAT) |
| $h_x$ (MxN values, or equilibrium) | 100*0.0, and $\theta = 0.4$ (steady state situation defined in THHFXFZ.DAT) |
| seepage face | 0 |

Weather data

irrigation rate 0

$T_p$ 0

$E_p$ 0

Timer control data

| $\Delta t_p$, $\Delta t_{max}$, $\Delta t_{min}$, $t_p$, $\zeta$, $m_t$ | (a) $10^{-3}$, 0.25, $10^{-3}$, 50.0, 0.01, 1.5; |
| | (b) $10^{-3}$, 0.025, $10^{-3}$, 50.0, 0.01, 1.5 |

Solution procedure n.a. (steady state)

Hysteresis n.a.

Solute transport

top boundary condition and boundary concentration $c_{top}$ no transport

bottom boundary condition and boundary conc. $c_{bottom}$ no transport
<table>
<thead>
<tr>
<th>left boundary condition and boundary concentration $c_{left}$</th>
<th>(a) no transport; (b) $c_{left} = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>right boundary condition and boundary conc. $c_{right}$</td>
<td>(a) $c_{right} = 0$; (b) no c gradient</td>
</tr>
<tr>
<td>$a_i$, $a_n$, $D_o$, $f_3$, $f_2$, $\theta_i$</td>
<td>2.0, 0.2, 1.64, 1.58, -0.17, 0.12</td>
</tr>
<tr>
<td>$C_o$ (MxN values)</td>
<td>1.0 mmol l$^{-1}$ (all nodes)</td>
</tr>
<tr>
<td><strong>Root data</strong></td>
<td></td>
</tr>
<tr>
<td>Root water uptake</td>
<td>n.a.</td>
</tr>
<tr>
<td>Root nutrient uptake</td>
<td>n.a.</td>
</tr>
<tr>
<td>Irrigation control unit</td>
<td>n.a. = not applicable</td>
</tr>
</tbody>
</table>
Input data used in example of Section 6.4. Similar as input data given in Appendix 6 of Heinen (1997).

<table>
<thead>
<tr>
<th>Basic units</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>length, time</td>
<td>cm, min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flow domain configuration</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$N, M$</td>
<td>15, 9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta x_i \ (N \ values)$</td>
<td>3<em>1.0, 2.0, 4</em>2.5, 2<em>5.0, 4</em>2.5, 5.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta z_j \ (M \ values)$</td>
<td>1.25, 2.5, 2<em>1.25, 2.5, 2</em>1.25, 2.5, 1.25</td>
<td></td>
<td></td>
</tr>
<tr>
<td>substrate</td>
<td>coarse sand, hydraulic properties listed in Table 4-6 of Heinen (1997)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>top boundary condition: $q_{top}, h_{top} \ (N \ values)$</th>
<th>$11<em>q_{top} = -E_p, 2</em>q_{top} = \text{irrigation rate} - E_p, 2*q_{top} = -E_p$</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>bottom boundary condition: $q_{bottom}, h_{bottom} \ (N \ values)$</td>
<td>$2*\text{seepage drainage, i.e } q_{bottom} = 0 \text{ or } h_{bottom} = 0, 13*q_{bottom} = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>left boundary condition: $q_{left}, h_{left} \ (N \ values)$</td>
<td>$9*q_{left} = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>right boundary condition: $q_{right}, h_{right} \ (M \ values)$</td>
<td>$9*q_{right} = 0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$h_{e} \ (MxN \ values, \ or \ equilibrium)$</td>
<td>equilibrium with $h = -8.5 \text{ cm at the bottom}$ (see Heinen (1997; Chapter 7.1) for reasons of this choice)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Weather data</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>irrigation rate</td>
<td>742<em>0 31</em>0.153 667<em>0 886</em>0 31<em>0.153 523</em>0 31<em>0.153 523</em>0 31<em>0.153 523</em>0 31<em>0.153 523</em>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1005<em>0 31</em>0.153 404<em>0 1095</em>0 31<em>0.153 314</em>0 31<em>0.153 314</em>0 31<em>0.153 314</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1440<em>0 788</em> 31<em>0.153 621</em>0 1440*0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1114<em>0 31</em>0.153 295<em>0 1440</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>846<em>0 31</em>0.153 563<em>0 1440</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>608<em>0 31</em>0.153 422<em>0 31</em>0.153 348*0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$T_p$</td>
<td>360<em>0 840</em>2.728<em>10^{-5} 240</em>0 360<em>0 840</em>4.533<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>4.854<em>10^{-5} 240</em>0 360<em>0 840</em>4.854<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>4.120<em>10^{-5} 240</em>0 360<em>0 840</em>4.120<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>4.182<em>10^{-5} 240</em>0 360<em>0 840</em>4.182<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>5.580<em>10^{-5} 240</em>0 360<em>0 840</em>5.580<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>9.393<em>10^{-5} 240</em>0 360<em>0 840</em>9.393<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E_p$</td>
<td>360<em>0 840</em>25.114<em>10^{-5} 240</em>0 360<em>0 840</em>23.566<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>30.163<em>10^{-5} 240</em>0 360<em>0 840</em>23.566<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>14.232<em>10^{-5} 240</em>0 360<em>0 840</em>14.232<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>9.812<em>10^{-5} 240</em>0 360<em>0 840</em>9.812<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>8.949<em>10^{-5} 240</em>0 360<em>0 840</em>8.949<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360<em>0 840</em>10.406<em>10^{-5} 240</em>0 360<em>0 840</em>10.406<em>10^{-5} 240</em>0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Timer control data</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t_p, \Delta t_{max}, \Delta t_{min}, t_f, \zeta, m_t$</td>
<td>0.1, 0.2, 10^{-15}, 17280, 0.01, 1.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<p>| Solution procedure | | | |</p>
<table>
<thead>
<tr>
<th>Procedure</th>
<th>ADI when completely unsaturated and ICCG when partially saturated; switch between the two at $h = -0.5$ cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_s$, max. # iterations</td>
<td>$10^3$, 20; convergence based on $K$ and $h$</td>
</tr>
<tr>
<td>ICCG: $e_s$, max. # iterations</td>
<td>$10^4$, 200</td>
</tr>
</tbody>
</table>

**Hysteresis**

<table>
<thead>
<tr>
<th>Initial $\kappa$ (MxN values), $e_s$</th>
<th>-2 (all nodes), 0.01</th>
</tr>
</thead>
</table>

**Solute transport**

<table>
<thead>
<tr>
<th>Top boundary condition and boundary concentration $c_{top}$</th>
<th>11°no flow, 2°inflow when fertigation occurs with $c_{top} = 15$ mmol l$^{-1}$, 2°no flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom boundary condition and boundary conc. $c_{bottom}$</td>
<td>2°solute outflow when drainage occurs (seepage drain) with solute flux density equal to drainage rate times local concentration, 13° no flow</td>
</tr>
<tr>
<td>Left boundary condition and boundary concentration $c_{left}$</td>
<td>9°no flow</td>
</tr>
<tr>
<td>Right boundary condition and boundary conc. $c_{right}$</td>
<td>9°no flow</td>
</tr>
</tbody>
</table>

| $a_u$, $a_p$, $D_u$, $f_u$, $f_p$, $\theta_1$ | 2.0, 0.2, 1.11·10$^{-3}$, 1.58, -0.17, 0.12                                           |
| $C_o$ (MxN values)                                | 15 mmol l$^{-1}$ (all nodes)                                                          |

**Root data**

<table>
<thead>
<tr>
<th>Root growth</th>
<th>yes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_{rcf}$ (MxN values) (cm cm$^{-3}$)</td>
<td>4°3.4027, 2°0.9060, 2°1.0587, 5.3033, 5.6787, 2°2.2437, 2°2.2770, 5.0550</td>
</tr>
<tr>
<td></td>
<td>4°3.4027, 2°0.9060, 2°1.0587, 5.3033, 5.6787, 2°2.2437, 2°2.2770, 5.0550</td>
</tr>
<tr>
<td></td>
<td>4°3.4027, 2°0.9060, 2°1.0587, 5.3033, 5.6787, 2°2.2437, 2°2.2770, 5.0550</td>
</tr>
<tr>
<td></td>
<td>4°2.44, 2°1.8383, 2°2.5173, 4.6547, 4.3220, 2°3.3817, 2°3.5573, 5.2860</td>
</tr>
<tr>
<td></td>
<td>4°2.44, 2°1.8383, 2°2.5173, 4.6547, 4.3220, 2°3.3817, 2°3.5573, 5.2860</td>
</tr>
<tr>
<td></td>
<td>4°2.44, 2°1.8383, 2°2.5173, 4.6547, 4.3220, 2°3.3817, 2°3.5573, 5.2860</td>
</tr>
<tr>
<td></td>
<td>4°0.7983, 2°0.7433, 2°0.7530, 1.0767, 0.4620, 2°0.6073, 2°0.6390, 0.3997</td>
</tr>
<tr>
<td></td>
<td>4°0.7983, 2°0.7433, 2°0.7530, 1.0767, 0.4620, 2°0.6073, 2°0.6390, 0.3997</td>
</tr>
<tr>
<td></td>
<td>4°0.7983, 2°0.7433, 2°0.7530, 1.0767, 0.4620, 2°0.6073, 2°0.6390, 0.3997</td>
</tr>
</tbody>
</table>

| $k$, $t'$: start time                          | 1.498·10$^{-4}$ cm min$^{-1}$, 30240 min, 17280 min                                 |

**Root water uptake**

| $K_s$, $R_p$, $a$, $h_{c,v}$ | 2.5·10$^{-3}$ cm min$^{-1}$, 0.017 cm (from Schwarz et al., 1995), 10, -9500 cm |

**Root nutrient uptake**

| $S_n$                              | 3·10$^{-5}$ mmol min$^{-1}$ (per plant; the three crop rows result in two plants) |

**Irrigation control unit**

| n.a.                               | n.a. = not applicable |
Input data used in example of Section 6.5.

<table>
<thead>
<tr>
<th>Basic units</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>length, time</td>
<td>cm, d</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flow domain configuration</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$N, M$</td>
<td>20, 24</td>
</tr>
<tr>
<td>$\Delta x_i \ (N \ values)$</td>
<td>$20 \times 10.0$</td>
</tr>
<tr>
<td>$\Delta z_j \ (M \ values)$</td>
<td>$9 \times 10.0, 5 \times 2.0, 10 \times 10.0$</td>
</tr>
<tr>
<td>substrate</td>
<td>zavelb7 from the 'Staringreeks' (Wösten et al., 1994)</td>
</tr>
<tr>
<td>top boundary condition: $q_{\text{top}}, h_{\text{top}} \ (N \ values)$</td>
<td>$3 \times h_{\text{top}} = 25.0 \ \text{cm}, 17 \times q_{\text{top}} = \text{irrigation rate}$</td>
</tr>
<tr>
<td>bottom boundary condition: $q_{\text{bottom}}, h_{\text{bottom}} \ (N \ values)$</td>
<td>$20 \times \text{no flow boundary: } q_{\text{bottom}} = 0$</td>
</tr>
<tr>
<td>left boundary condition: $q_{\text{left}}, h_{\text{left}} \ (M \ values)$</td>
<td>$5 \times q_{\text{left}} = 0, 9 \times \text{seepage face, i.e. } q_{\text{left}} = 0 \ or \ h_{\text{left}} = 0, h_{\text{left}} = 5.0, h_{\text{left}} = 15.0, 8 \times q_{\text{left}} = 0$</td>
</tr>
<tr>
<td>right boundary condition: $q_{\text{right}}, h_{\text{right}} \ (M \ values)$</td>
<td>$24 \times \text{no flow boundary } q_{\text{right}} = 0$</td>
</tr>
<tr>
<td>$h_j \ (M \times N \ values, \ or \ equilibrium)$</td>
<td>vertical equilibrium with $h$ at bottom equal to 100</td>
</tr>
<tr>
<td>seepage face</td>
<td>1: see left boundary conditions</td>
</tr>
</tbody>
</table>

| Weather data                  |                  |
| irrigation rate               | $2.5 \ \text{cm \ d}^{-1} \ (\text{constant})$ |
| $T_p$                          | 0                |
| $E_p$                          | 0                |

| Timer control data            |                  |
| $\Delta t_p, \Delta t_{\text{max}}, \Delta t_{\min}, t_p, \zeta, m_t$ | $10^5, 0.25, 10^{-5}, 10.0, 0.01, 1.5$ |

| Solution procedure            |                  |
| procedure                     | ICCG             |
| $e_p, \text{max. \ # \ iterations}$ | $10^4, 20$       |
| ICCG: $e_p, \text{max. \ # \ iterations}$ | $10^6, 200$      |

| Hysteresis                     | n.a.             |

<p>| Solute transport               |                  |
| top boundary condition and boundary concentration $c_{\text{top}}$ | $3 \times \text{possible outflow with } c_{\text{top}} = 0, 17 \times \text{no flow}$ |
| bottom boundary condition and boundary conc. $c_{\text{bottom}}$ | $20 \times \text{no flow}$ |</p>
<table>
<thead>
<tr>
<th><strong>left boundary condition and boundary concentration</strong> $c_{\text{left}}$</th>
<th>5<em>no flow, 9</em>possible seepage outflow, with $c_{\text{left}} = 0$, 2<em>possible outflow with $c_{\text{left}} = 0$, 8</em>no flow</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>right boundary condition and boundary conc.</strong> $c_{\text{right}}$</td>
<td>24*no flow</td>
</tr>
<tr>
<td>$a_r$, $a_l$, $D_o$, $f_r$, $f_l$, $\theta_l$</td>
<td>2.0, 0.2, 1.64, 1.58, -0.17, 0.12</td>
</tr>
<tr>
<td>$C_0$ (MxN values)</td>
<td>10.0 mmol l$^{-1}$ (all nodes inside flow domain)</td>
</tr>
<tr>
<td><strong>Root data</strong> n.a.</td>
<td></td>
</tr>
<tr>
<td><strong>Root water uptake</strong> n.a.</td>
<td></td>
</tr>
<tr>
<td><strong>Root nutrient uptake</strong> n.a.</td>
<td></td>
</tr>
<tr>
<td><strong>Irrigation control unit</strong> n.a.</td>
<td></td>
</tr>
<tr>
<td>n.a. = not applicable</td>
<td></td>
</tr>
</tbody>
</table>
Input data used in example of Section 6.6.

<table>
<thead>
<tr>
<th>Basic units</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>length, time</td>
<td>cm, d</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flow domain configuration</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$N, M$</td>
<td>15, 9</td>
</tr>
<tr>
<td>$\Delta x_i$ ($N$ values)</td>
<td>3<em>1.0, 2.0, 4</em>2.5, 2<em>5.0, 4</em>2.5, 5.0</td>
</tr>
<tr>
<td>$\Delta z_i$ ($M$ values)</td>
<td>1.25, 2.5, 2<em>1.25, 2.5, 2</em>1.25, 2.5, 1.25</td>
</tr>
<tr>
<td>substrate</td>
<td>coarse sand, hydraulic properties listed in Table 4-6 of Heinen (1997)</td>
</tr>
<tr>
<td>top boundary condition: $q_{top}, h_{top}$ ($N$ values)</td>
<td>11<em>q_{top} = -E_p, 2</em>q_{top} = irrigation rate - E_p, 2*q_{top} = -E_p</td>
</tr>
<tr>
<td>bottom boundary condition: $q_{bottom}, h_{bottom}$ ($N$ values)</td>
<td>2<em>seepage drainage, i.e. q_{bottom} = 0 or h_{bottom} = 0, 13</em>q_{bottom} = 0</td>
</tr>
<tr>
<td>left boundary condition: $q_{left}, h_{left}$ ($M$ values)</td>
<td>9*q_{left} = 0</td>
</tr>
<tr>
<td>right boundary condition: $q_{right}, h_{right}$ ($M$ values)</td>
<td>9*q_{right} = 0</td>
</tr>
<tr>
<td>$h_0$ ($MxN$ values, or equilibrium)</td>
<td>equilibrium with $h = -8.5$ cm at the bottom (see Heinen (1997; Chapter 7.1) for reasons of this choice)</td>
</tr>
<tr>
<td>seepage face</td>
<td>seepage drain at bottom, see bottom boundary conditions</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Weather data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>irrigation rate</td>
<td>0</td>
</tr>
<tr>
<td>$T_p$</td>
<td></td>
</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
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<td>360*0</td>
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</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
</tr>
<tr>
<td>$E_p$</td>
<td></td>
</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
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<td>360*0</td>
<td>240*0</td>
</tr>
<tr>
<td>360*0</td>
<td>240*0</td>
</tr>
</tbody>
</table>

| Timer control data                              |                  |
| $\Delta t_p, \Delta t_{max}, \Delta t_{min}$, $t_p$, $\zeta$, $m_t$ | 0.1, 15, 10^{-15}, 17280, 0.01, 1.5 |

<p>| Solution procedure                              |                  |
| procedure                                       | ICCG            |
| $\epsilon_s$, max. # iterations                | $10^{4}, 20$; convergence based on $K$ and $h$ |
| ICCG: $\epsilon_p$, max. # iterations          | $10^{3}, 200$   |
| Hysteresis n.a. (only drying out)               |                  |</p>
<table>
<thead>
<tr>
<th>Solute transport</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>top boundary condition and boundary concentration $c_{\text{top}}$</td>
<td>no transport</td>
</tr>
<tr>
<td>bottom boundary condition and boundary conc. $c_{\text{bottom}}$</td>
<td>no transport</td>
</tr>
<tr>
<td>left boundary condition and boundary concentration $c_{\text{left}}$</td>
<td>no transport</td>
</tr>
<tr>
<td>right boundary condition and boundary conc. $c_{\text{right}}$</td>
<td>no transport</td>
</tr>
</tbody>
</table>

| $a$, $a_n$, $D_w, f_s, f_p, \theta_i, D_o$ | 2.0, 0.2, 1.58, -0.17, 0.12 |
| 1.64 (NO$_3$), 1.69 (K), 1.74 (P), 0.685 (Ca), 0.610 (Mg), 0.920 (S), 1.76 (Cl), 1.15 (Na) |

| $C_o$ (MxN values) | 21.0 (NO$_3$), 11.2 (K), 4.0 (P), 4.6 (Ca), 1.0 (Mg), 1.4 (S), 0.5 (Cl), 0.03 (Na) (all nodes) |

<table>
<thead>
<tr>
<th>Root data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Root growth</td>
<td>yes</td>
</tr>
<tr>
<td>$L_{\text{root}}$ (MxN values)</td>
<td>4<em>3.4927, 2</em>0.9060 2<em>1.0587, 5.3033, 5.6787 2</em>2.2437, 2*2.2770, 5.0550</td>
</tr>
<tr>
<td>$4\times 3.4927, 2\times 0.9060, 2\times 1.0587, 5.3033, 5.6787, 2\times 2.2437, 2\times 2.2770, 5.0550$</td>
<td></td>
</tr>
<tr>
<td>4<em>3.4927, 2</em>0.9060, 2<em>1.0587, 5.3033, 5.6787, 2</em>2.2437, 2*2.2770, 5.0550</td>
<td></td>
</tr>
<tr>
<td>4<em>2.44, 2</em>1.8383, 2<em>2.5173, 4.6547, 4.3220, 2</em>3.3817, 2*3.5573, 5.2660</td>
<td></td>
</tr>
<tr>
<td>4<em>2.44, 2</em>1.8383, 2<em>2.5173, 4.6547, 4.3220, 2</em>3.3817, 2*3.5573, 5.2660</td>
<td></td>
</tr>
<tr>
<td>4<em>2.44, 2</em>1.8383, 2<em>2.5173, 4.6547, 4.3220, 2</em>3.3817, 2*3.5573, 5.2660</td>
<td></td>
</tr>
<tr>
<td>4<em>0.7983, 2</em>0.7433, 2<em>0.7530, 1.0767, 0.4620, 2</em>0.6073, 2*0.6390, 0.3997</td>
<td></td>
</tr>
<tr>
<td>4<em>0.7983, 2</em>0.7433, 2<em>0.7530, 1.0767, 0.4620, 2</em>0.6073, 2*0.6390, 0.3997</td>
<td></td>
</tr>
</tbody>
</table>

| $k_t, t^*$, start time | 0.2157, 21, 13 |

<table>
<thead>
<tr>
<th>Root water uptake</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_s, R_w, a, h_{o2}, a_n, h_{or}$</td>
<td>3.6 $10^6$, 0.017, 10, -9500, 0.9, 0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Root nutrient uptake</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_{sr}$</td>
<td>9.36 $10^3$ (NO$_3$), 5.47 $10^2$ (K), 5.76 $10^2$ (P), 6.05 $10^2$ (Ca), 3.31 $10^2$ (Mg), 2.02 $10^2$ (S), 1.73 $10^2$ (Cl), 0.0 (Na) (per plant; the three crop rows result in two plants)</td>
</tr>
</tbody>
</table>

| Irrigation control unit n.a. |   |
|-------------------------------| n.a. = not applicable |
Appendix 4  Steady-state solution for water flow with a 2-D exponentially distributed sink

The governing equation is given by Eq. [212] in the main text. The exponential $K(h)$ relationship of Gardner (1958) is used (Eq. [213] in main text), and a double exponential distribution of the sink term is proposed (Eq. [218] in the main text). The boundary conditions are given as Eqs [13]-[16] in the main text. In this Appendix an analytical solution for the steady state problem is derived.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left( K(h) \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial z} \left( K(h) \frac{\partial h}{\partial z} \right) - \frac{\partial K(h)}{\partial z} = S_w = 0. \quad [A4-1]$$

The exponential $K(h)$ relationship of Gardner (1958) is used

$$K(h) = K_s e^{-\alpha h}, \quad [A4-2]$$

with $\alpha$ not to be confused with the $\alpha$ occurring in the Van Genuchten-Mualem relationships. For convenience the independent variables are made dimensionless by

$$\zeta = \frac{\pi}{X} (Z - z), \quad [A4-3]$$

and

$$\xi = \frac{\pi}{X} (X - x). \quad [A4-4]$$

Then the following system of equations is obtained

$$\frac{\partial^2 K}{\partial \xi^2} + \frac{\partial^2 K}{\partial \zeta^2} + \lambda \frac{\partial K}{\partial \zeta} = -S_w e^{\alpha \xi} e^{b \xi} = 0, \quad [A4-5]$$

with the new boundary conditions given by

$$\xi = 0 \quad \frac{\partial K}{\partial \xi} = 0, \quad [A4-6]$$

$$\xi = \pi \quad \frac{\partial K}{\partial \xi} = 0, \quad [A4-7]$$

$$\zeta = \zeta_1, \quad \frac{\partial K}{\partial \zeta} = -\lambda K, \quad [A4-8]$$

$$\zeta = 0, \quad K = K_s, \quad [A4-8]$$

where
\[ A_o = \frac{W^2}{\pi^2} \alpha S_o e^{-pX} e^{-qZ}, \quad [A4-9] \]

\[ a = \frac{pX}{\pi}, \quad b = \frac{qX}{\pi}, \quad [A4-10] \]

and

\[ \lambda = \frac{X}{\pi}. \quad [A4-11] \]

To solve this system the finite cosine transform (Churchill 1972, page 355-356) with respect to \( \zeta \) is employed. This transform of a function \( F(x) \) is defined as

\[ C_n[F(x)] = f_\zeta(n) = \int_0^\pi F(x) \cos(nx) \, dx, \quad n=0,1,2,..., \quad [A4-12] \]

with inverse

\[ F(x) = \frac{f_\zeta(0)}{\pi} + \frac{2}{\pi} \sum_{n=1}^\infty f_\zeta(n) \cos(nx), \quad [A4-13] \]

and with the operational property

\[ C_n[F"(x)] = -n^2 f_\zeta(n) - F'(0) + (-1)^n F'(\pi). \quad [A4-14] \]

Under this transformation the sink term transforms into

\[ C_n[A_o e^{a\zeta} e^{b\zeta}] = A_o e^{b\zeta} \int_0^\pi e^{a\zeta} \cos(n\zeta) \, d\zeta = A_o e^{b\zeta} \frac{a \left( e^{a\pi}(-1)^n - 1 \right)}{n^2 + a^2} = A_o e^{b\zeta} \phi(n). \quad [A4-15] \]

Using the property Eq. [A4-14] for \( n = 0 \), Eq. [A4-5] transforms into

\[ \frac{d^2 k}{d \zeta^2} + \lambda \frac{d k}{d \zeta} = A_o \phi(0) e^{b\zeta}, \quad [A4-16] \]

where

\[ k = C_0(K). \quad [A4-17] \]

with the solution

\[ k(0, \zeta) = B_1 e^{-\lambda \zeta} + B_2 + \frac{A_o \phi(0)}{b (b + \lambda)} e^{b \zeta}. \quad [A4-18] \]

The boundary conditions Eqs. [A4-7] and [A4-8] transform into
\[ \zeta = \zeta_1, \quad \frac{d k}{d \zeta} = -\lambda k, \quad [A4-19] \]

and

\[ \zeta = 0, \quad k = \pi K_s. \quad [A4-20] \]

From Eq. [A4-19] it follows

\[ B_2 = -\frac{A_0 \phi(0)}{b \lambda} e^{b \zeta}, \quad [A4-21] \]

and from Eq. [A4-20]

\[ B_1 = \pi K_s - \frac{A_0 \phi(0)}{b (b + \lambda)} + \frac{A_0 \phi(0)}{b \lambda} e^{b \zeta}. \quad [A4-22] \]

Note that

\[ \lim_{p \to 0} \frac{k(0, \zeta)}{\pi} = -\frac{A_0}{b \lambda} e^{b \zeta} + \left( K_s - \frac{A_0}{b (b + \lambda)} + \frac{A_0}{b \lambda} \right) e^{-\lambda \zeta} + \frac{A_0}{b (b + \lambda)} e^{b \zeta}, \quad [A4-23] \]

is the solution of Eq. [A4-5] when water uptake in x-direction is uniform. For other values of n Eq. [A4-5] now transforms into

\[ -n^2 k + \frac{d^2 k}{d \zeta^2} + \lambda \frac{d k}{d \zeta} = A_0 e^{b \zeta} \phi(n), \quad [A4-24] \]

with the solution

\[ k(n, \zeta) = B_3 e^{m_3 \zeta} + B_4 e^{m_4 \zeta} - \frac{A_0 e^{b \zeta} \phi(n)}{n^2 - b (b + \lambda)}, \quad [A4-25] \]

where

\[ m_{1,2} = \frac{-\lambda \pm \sqrt{\lambda^2 + 4 n^2}}{2}. \quad [A4-26] \]

The boundary conditions Eqs. [A4-7] and [A4-8] for \( n = 1, 2, \ldots \) transform into

\[ \zeta = \zeta_1, \quad \frac{d k}{d \zeta} = -\lambda k, \quad [A4-27] \]

and

\[ \zeta = 0, \quad k = 0. \quad [A4-28] \]

From Eqs. [A4-27] and [A4-28] it follows
\[ B_3 = \frac{A_0 \phi(n)}{n^2 - b(b + \lambda)} \frac{e^{b \zeta/(b + \lambda)} - e^{m_2 \zeta/(m_2 + \lambda)}}{e^{m_1 \zeta/(m_1 + \lambda)} - e^{m_3 \zeta/(m_3 + \lambda)}} , \]  

[A4-29]

and

\[ B_4 = -\frac{A_0 \phi(n)}{n^2 - b(b + \lambda)} \frac{e^{b \zeta/(b + \lambda)} - e^{m_2 \zeta/(m_2 + \lambda)}}{e^{m_1 \zeta/(m_1 + \lambda)} - e^{m_3 \zeta/(m_3 + \lambda)}} , \]  

[A4-30]

So that the complete solution is given as

\[ K(z, \xi) = B_2 e^{-i \zeta/\beta} + B_4 e^{-i (b + \lambda)/(b + \lambda)} + 2 \sum_{n=1}^{\infty} \left( B_3 e^{m_1 \zeta/(m_1 + \lambda)} + B_5 e^{m_3 \zeta/(m_3 + \lambda)} \right) \cos(n \xi) + \]  

[A4-31]

\[-\frac{A_0 e^{b \zeta}}{\pi} - \sum_{n=1}^{\infty} \frac{\phi(n)}{n^2 - b^2} \cos(n \xi) , \]

where for convenience

\[ \beta^2 = b(b + \lambda) . \]  

[A4-32]

One can use a convolution theorem to evaluate the third term of the RHS of Eq. [A4-31]. Now (Churchill 1972, table B.2, entry 20)

\[ C_n^{-1} \left\{ \frac{1}{n^2 - \beta^2} \right\} = -\frac{\cos(\beta(\pi - \xi))}{\beta \sin(\pi \beta)} = H(\xi) , \]  

[A4-33]

and

\[ C_n^{-1}(\phi(n)) = e^{a \zeta} = F(\zeta) . \]  

[A4-34]

The inverse transform can then be given as the sum of four integrals (Churchill, 1972, page 358, (9) and (10)) these being respectively

\[ l_1 = \int_{0}^{\xi} F(r) H(\xi - r) \, dr , \]  

[A4-35]

\[ l_2 = \int_{\zeta}^{\infty} F(r) H(r - \xi) \, dr , \]  

[A4-36]

\[ l_3 = \int_{0}^{\pi - \zeta} F(r) H(r + \xi) \, dr , \]  

[A4-37]
and

\[ I_n = \int_{\pi-\xi}^{\pi} F(r) H(2\pi-r-\xi) \, dr. \]  
[A4-38]

Performing the integrations and summing the results yields

\[ \sum_{n=0}^{\infty} \frac{\phi(n)}{n^2 - \beta^2} \cos(n\xi) = \sum_{i=1}^{4} I_1 = \frac{a \cos(\beta(\pi-\xi)) - a e^{\pi a} \cos(\beta\xi) - e^{a\xi} \sin(\pi\beta)}{(a^2 + \beta^2) \sin(\pi\beta)} = G(\xi). \]  
[A4-39]

But from Eq. [A4-13]

\[ G(\xi) = \frac{\phi(0)}{\pi \beta^2} + 2 \sum_{n=1}^{\infty} \frac{\phi(n)}{n^2 - \beta^2} \cos(n\xi), \]  
[A4-40]

or

\[ \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\phi(n)}{n^2 - \beta^2} \cos(n\xi) = \frac{\phi(0)}{\pi \beta^2} + G(\xi). \]  
[A4-41]

So ultimately

\[ K(\xi, \zeta) = \frac{A_0 \phi(0)}{\pi b \lambda} + \left( K_1 + \frac{2 A_0 \phi(0)}{\pi \beta} + \frac{A_0 \phi(0) e^{b \zeta}}{\pi b \lambda} \right) e^{-\lambda \zeta} + \]

\[ - A_0 e^{b \zeta} \frac{a \cos(\beta(\pi-\xi)) - a e^{\pi a} \cos(\beta\xi) - e^{a\xi} \sin(\pi\beta)}{(a^2 + \beta^2) \sin(\pi\beta)} + \]

\[ + \sum_{n=1}^{\infty} A_0 \phi(n) \left\{ \left[ \frac{e^{b \zeta} (b + \lambda) - e^{m_2 \zeta} (m_2 + \lambda)}{(n^2 - \beta^2) \left( e^{m_2 \zeta} (m_2 + \lambda) - e^{m_1 \zeta} (m_1 + \lambda) \right)} \right] e^{m_1 \zeta} - \left( e^{b \zeta} (b + \lambda) - e^{m_1 \zeta} (m_1 + \lambda) \right) \right\}. \]  
[A4-42]
List of symbols

The following notation conventions were used:

- **Matrix**: BOLD, ROMAN, CAPITAL
- **Vector**: bold, roman, small
- **Scalar**: italic
- **Integrated scalar**: italic and bold
- **Functions, operators**: roman
- **Numbers**: roman

The basic SI dimensions 1, A, L, M, T, m and Θ represent dimensionless, strength of current, length, mass, time, molar amount of a species and temperature, respectively, while the deduced dimensions J, V and Ω represent energy, voltage and resistance, respectively (NEN 999, 1977).

The list below presents: the symbol, its description, its dimension, and the equation number or section number of first occurrence. Not all variables appearing in Appendix 4 are explained.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Dimension</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Coefficient matrix</td>
<td>L²T⁻¹</td>
<td>[114]</td>
</tr>
<tr>
<td>A⁻¹</td>
<td>Inverse of A</td>
<td>L²T⁻¹</td>
<td>[115]</td>
</tr>
<tr>
<td>A</td>
<td>Coefficient referring to central node</td>
<td>L²T⁻¹</td>
<td>[74,78]</td>
</tr>
<tr>
<td>A*</td>
<td>Double exponentially distributed sink term</td>
<td>L⁰T³⁻¹</td>
<td>[212]</td>
</tr>
<tr>
<td>A₀*</td>
<td>Constant in double exponential A* expression</td>
<td>L¹L⁻³T⁻¹</td>
<td>[218,219,220]</td>
</tr>
<tr>
<td>A₀</td>
<td>Dimensionless A₀</td>
<td>1</td>
<td>[221-225,A4-9]</td>
</tr>
<tr>
<td>Aᵦ</td>
<td>Coefficient referring to C of central node</td>
<td>L²T⁻¹</td>
<td>[77]</td>
</tr>
<tr>
<td>Aₑ</td>
<td>K-geometry coefficient between central node (I,J) and its eastern neighbour node (I+1,J)</td>
<td>L²T⁻¹</td>
<td>[74,75]</td>
</tr>
<tr>
<td>Aᵦ</td>
<td>K-geometry coefficient between central node (I,J) and its northern neighbour node (I,J-1)</td>
<td>L²T⁻¹</td>
<td>[74,75]</td>
</tr>
<tr>
<td>Aₛ</td>
<td>K-geometry coefficient between central node (I,J) and its southern neighbour node (I,J+1)</td>
<td>L²T⁻¹</td>
<td>[74,75]</td>
</tr>
<tr>
<td>Aₛ</td>
<td>K-geometry coefficient between central node (I,J) and its western neighbour node (I-1,J)</td>
<td>L²T⁻¹</td>
<td>[74,75,79]</td>
</tr>
<tr>
<td>Aᵦ</td>
<td>Parameter in expression for activity coefficient</td>
<td>M⁰⁸⁵m⁰⁵</td>
<td>[37,38]</td>
</tr>
<tr>
<td>B</td>
<td>Boundary condition function</td>
<td>1</td>
<td>[8]</td>
</tr>
<tr>
<td>B₁</td>
<td>Dummy term</td>
<td>L¹T¹</td>
<td>[221,222]</td>
</tr>
<tr>
<td>B₂</td>
<td>Dummy term</td>
<td>L¹T¹</td>
<td>[221,223]</td>
</tr>
<tr>
<td>B₃</td>
<td>Dummy term</td>
<td>L¹T¹</td>
<td>[221,224]</td>
</tr>
<tr>
<td>B₄</td>
<td>Dummy term</td>
<td>L¹T¹</td>
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$D_w$ Water diffusivity = $K(\partial/\partial c(h))$

$D_{xx}$ Dispersion/diffusion coefficient for transport in x direction due to a gradient of c in the x-direction

$D_{xz}$ Dispersion/diffusion coefficient for transport in x direction due to a gradient of c in the z-direction

$D_{zx}$ Dispersion/diffusion coefficient for transport in z direction due to a gradient of c in the x-direction

$D_{zz}$ Dispersion/diffusion coefficient for transport in z direction due to a gradient of c in the z-direction

$EC$ Electrical conductivity

$F_0$ Faraday’s constant

$F_0$ Fourier number

$G$ Dimensionless geometry function

$G_0$ Dimensionless geometry function, special case of $G$

$H$ Hydraulic head

$I$ Index of column number

$l$ Ionic strength

$l_0$ Incomplete beta function of order $\eta$

$L$ Index of row number

$K$ Hydraulic conductivity

$K_{r}$ Root hydraulic conductance

$K$ at $z = Z$

$K_r$ Relative $K$

$K_s$ $K$ at saturation

$K_x$ $K$ in x-direction

$K_{x,ij}$ $K$ at $x_{ij}$

$K_{x,ij}$ $K$ at $x_{ij}$

$K_z$ $K$ in z-direction

$K_{z,ij}$ $K$ at $z_{ij}$

$K_{z,ij}$ $K$ at $z_{ij}$

$K_r^*$ Specified $K$ normal to the boundary $\Gamma$

$L$ Cholesky lower triangular matrix

$L^T$ Transpose of $L$

$L_D$ Single dispersivity

$L_{rv}$ Root length density

$M$ Number of rows

$N$ Number of columns

$N_0$ Avogadro’s number

$P_e$ Peclet number

$P_d$ Domain dependence factor

$Q$ Total density of nutrient per unit volume of substrate

$Q_m$ Total amount of nutrient

$Q_{mo}$ Initial value of $Q_m$

$R$ Radial coordinate

$R_o$ Root radius

$R_{p}$ Radius of porous medium surrounding a root

$R_g$ Universal gas constant

$S_e$ Reduced volumetric water content

$S_s$ Sink strength for solute; or root nutrient uptake rate

$S_{sm}$ Maximum possible root nutrient uptake rate per unit surface area of substrate

$S_{nr}$ Required nutrient uptake rate

$S_{nr,c}$ Required nutrient uptake per unit root length

$S_{sw}$ Sink strength for water or root water uptake rate

$T$ Transpiration rate

$T$ Temperature

$T_d$ Dummy term

$T_d$ Dummy term

$T_d$ Dummy term

$T_d$ Dummy term

$\Theta$ [38,39]

1 [195,196]

1 [195,197]

1 [195,198]

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\( \theta_{m,d} \) \( \theta \) of main drying curve \( \text{L}^3 \text{L}^{-3} \) [190]

\( \theta_w \) \( \theta \) of scanning wetting curve \( \text{L}^3 \text{L}^{-3} \) [189,190]

\( \theta_{m,w} \) \( \theta \) of main wetting curve \( \text{L}^3 \text{L}^{-3} \) [A2-1]

\( \theta_a \) \( \theta \) at reversal point \( \text{L}^3 \text{L}^{-3} \) [A2-1]

\( \Delta \theta \) Change in \( \theta \) of the latest drying process \( \text{L}^3 \text{L}^{-3} \) [A2-1]

\( \Delta \theta_b \) \( \Delta \theta \) in the absence of blockage of air access \( \text{L}^3 \text{L}^{-3} \) [A2-1]

\( i \) Matrix index \( 1 \) [129]

\( k \) Matrix index \( 1 \) [129]

\( k^* \) Hysteresis direction pointer \( 1 \) [201,202]

\( k_h \) Hysteresis pointer \( 1 \) [202]

\( \lambda \) Local iteration counter in conjugate gradient iterative solution procedure (Eq. [134] only) \( 1 \) [134]

\( \lambda \) Curve-shape parameter \( 1 \) [183]

\( \lambda \) Some dimensionless profile width \( 1 \) [A4-11]

\( \mu \) Boundary condition parameter \( \text{L}^{-1} \) [8]

\( \mu_m \) Ionic mobility \( \text{L}^2 \text{T}^{-4} \text{V}^{-1} \) [35]

\( v \) Boundary condition parameter \( 1 \) [8]

\( \xi \) Dimensionless \( x \) coordinate \( 1 \) [221,226,A4-4]

\( \pi \) Number pi \( 1 \) [19]

\( \rho \) Dimensionless radius of soil cylinder surrounding a root \( 1 \) [21]

\( \rho_n \) Density of solvent \( \text{L}^{-3} \text{M}^{-1} \) [35]

\( \sigma \) Dimensionless root water uptake rate \( 1 \) [48,49]

\( \sigma \) Dummy variable \( L \) [205,210]

\( \sigma_R \) Reflection coefficient for solutes at the root membrane \( 1 \) [20]

\( \tau \) Tortuosity factor \( 1 \) [33,34]

\( \tau \) Dummy variable \( L \) [205,210]

\( \phi \) Matric flux potential \( \text{L}^T \) [7]

\( \phi \) Some analytical solution function \( 1 \) [209,210]

\( \phi(n) \) Some dimensionless parameter \( 1 \) [221,A4-15]

\( \phi \) Average matric flux potential \( \text{L}^T \) [22,23]

\( \phi_n \) Matric flux potential at root-porous medium interface \( \text{L}^T \) [22]

\( \psi \) Some analytical solution function \( 1 \) [204,205]

---

**Mathematical operators**

\[ \cos \] Cosine

\[ \text{d} \] Derivative operator

\[ \text{e, exp} \] Natural base

\[ \text{erfc} \] Complementary error function

\[ \ln \] Natural logarithm

\[ \text{max} \] Operator yielding the maximum value in argument list

\[ \text{min} \] Operator yielding the minimum value in argument list

\[ \nabla \] Gradient operator

\[ \nabla \cdot \] Divergence operator

\[ \partial \] Partial derivative operator

\[ \partial / \partial n \] The exterior normal derivative operator

\[ \mathcal{Q} \] Some differential operator (Subsection 3.2.1)

\[ | \eta | \] Represents the absolute value of argument \( \eta \)

\( \Delta \) Small increment

\{,\} In-product of two vectors
### Abbreviations

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<th>Description</th>
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<td>DLO Research Institute for Agrobiology and Soil Fertility (DLO Instituut voor Agrobiologie en Bodemvruchtbaarheid)</td>
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<tr>
<td>ADI</td>
<td>Alternating Direction Implicit</td>
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<tr>
<td>CV</td>
<td>Control Volume</td>
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<td>Incomplete Cholesky-Conjugate Gradient</td>
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