FUSSIM2 version 5. New features and updated user's guide

New features and updated user's guide

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ABSTRACT

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FUSSIM2 is a two-dimensional simulation model for describing movement of water, solute transport and root uptake of water and nutrients in partially saturated porous media. It has been documented in 1998 (Heinen and de Willigen, QASA Report 20, AB-DLO & PE, Wageningen, The Netherlands). Since then new features have been included that are described in the current report. The new features include: extension to the van Genuchten – Mualem description of the physical properties of the porous medium, reduction of evaporation of water at the soil surface, runoff, the Vimoke drain concept, P-adsorption and P-fixation, non-zero sink nutrient uptake, root growth described as a diffusion process, nitrification and denitrification, soil temperature. Furthermore, a version in cylindrical coordinates is available, FUSSIM2 is coupled with the organic matter model MOTOR, and a expo-lineair growth and demand module is included in FUSSIM2 for special situations. This report includes an updated users' guide.

Keywords: drain, evaporation, nitrate, radial transport, root growth, root uptake, phosphate, soil temperature, solute transport, two-dimensional simulation model, Vimoke, water flow denitrification, nitrification

Alterra is the amalgamation of the Institute for Forestry and Nature Research (IBN) and the Winand Staring Centre for Integrated Land, Soil and Water Research (SC). The merger took place on 1 January 2000.

Contents

Preface

This report was written within project 10198 ('*Verbetering en toetsing FUSSIM2*') as part of the research program 317 ('*Dynamiek en beheer van nutriënten*') It was financed by "*Dienst Wetenschap en Kennisoverdracht*" (DWK) of the Dutch Ministry of Agriculture, Fisheries and Nature Management (LNV). It is an update of a previous description of FUSSIM2, a two-dimensional simulation model for describing water movement, solute transport and root uptake of water and nutrients in partially saturated porous media (Heinen and de Willigen, 1998. Quantitative Approaches in Systems Analysis No. 20, AB-DLO and PE, Wageningen, The Netherlands). The last chapter is a user's guide for the model.

At each chapter it is indicated who the responsible authors are. Authors who contributed are: M. Heinen, P. de Willigen, F.B.T. Assinck, J.A. de Vos (all Alterra), and J.G. Conijn (Plant Research International).

Summary

FUSSIM2 is a two-dimensional simulation model for describing water movement, solute transport and root uptake of water and nutrients in partially saturated porous media. It was documented by Heinen and de Willigen in 1998 (Quantitative Approaches in Systems Analysis No. 20, AB-DLO and PE, Wageningen, The Netherlands). Since then there have been additions to FUSSIM2, which are described in this report. Also the user's guide needed to be updated due to these additions, and forms the last chapter of this report.

The new features include: extension to the van Genuchten – Mualem description of the physical properties of the porous medium, reduction of evaporation of water at the soil surface, runoff, the Vimoke drain concept, P-adsorption and P-fixation, non-zero sink nutrient uptake, root growth described as a diffusion process, nitrification and denitrification, soil temperature. Furthermore, a version in cylindrical coordinates is available, FUSSIM2 is coupled with the organic matter model MOTOR, and a expo-lineair growth and demand module is included in FUSSIM2 for special situations.

1 Introduction

FUSSIM2 is a two-dimensional simulation model for describing water movement, solute transport and root uptake of water and nutrients in partially saturated porous media. It has been documented by Heinen and de Willigen (1998). Since then, several additions have been implemented in the code, and we feel obliged to describe them in this report. We have decided to describe each feature in a separate chapter. The responsible author(s) for each chapter are given at the beginning of each chapter.

In this report the following chapters are present

2	FUSSIM2 for 1-dimensional cases
3	Cylindrical coordinates: FUSSIMR
4	Extension to the van Genuchten-Mualem description of the hydraulic properties in FUSSIM2
5	From potential to actual evaporation of water at the soil surface
6	Infiltration and runoff of water at the soil surface
7	Drain according to the Vimoke concept in FUSSIM2
8	P-adsorption and P-fixation in FUSSIM2
9	Non-zero sink nutrient uptake
10	Expo-linear growth and demand
11	Root growth described as a diffusion process
12	Nitrification and denitrification module NITDEN
13	Soil temperature (1-D)
14	Coupling with MOTOR
15	User's guide

The last chapter is the update of the user's guide as given by Heinen and de Willigen (1998). Each chapter can be considered as separate units. They have their own usage of symbols and their own list of references.

In general, since the previous description of FUSSIM2 (Heinen and de Willigen, 1998) the model has been used extensively. In most cases it was coupled with plant growth models. For this purpose use was made of the FSE4 shell (Rappoldt, 2001) software, which was specifically made for coupling existing models. As such, FUSSIM2 is no longer a stand-alone model, as it has to run under FSE4 (or any other synchronization main program or shell). Under FSE4, FUSSIM2 can be run as a single model. However, the user needs to take care of any required plant data in that case. For this situation the user can choose to use the build-in expo-linear crop model (chapter 10).

1.1 References

Heinen M. and P. de Willigen, 1998. FUSSIM2 A two-dimensional simulation model for water flow, solute transport and root water and root nutrient uptake in unsaturated and partly unsaturated porous media. Quantitative Approaches in

Systems Analysis No. 20, DLO Research Institute for Agrobiology and Soil Fertility and the C.T. de Wit Graduate School for Production Ecology, Wageningen, The Netherlands, 140 p.

Rappoldt C, 2001. Description of the FSE4 shell. Internal Report, Alterra, Wageningen, in preparation.

2 FUSSIM2 for 1-dimensional cases

Marius Heinen

2.1 Introduction

FUSSIM2 can easily be used for 1-dimensional studies by setting the input parameter NC equal to one. The code of FUSSIM2 has been adapted such that this case can be handled correctly. For the 1-D case, the matrix problem (Eq. [114] of Heinen and de Willigen, 1998) consists of a tri-diagonal coefficient matrix **A**, which can be easily solved (e.g. Press *et al.*, 1992). The main diagonal contains the coefficients of the central CV's, and the upper and lower diagonals contain the coefficients referring to the northern and southern neighbors.

It is also possible to consider several columns as independent 1-dimensional columns, i.e. there will be no flow between the columns. Setting up the equations for all columns again yields a tri-diagonal system which can be solved as described above. This option can be achieved by setting ISOLVE < 0 (see chapter 15). This option was implemented for a special case study, but it is still available for the future.

2.2 References

Heinen M. and P. de Willigen, 1998. FUSSIM2 A two-dimensional simulation model for water flow, solute transport and root water and root nutrient uptake in unsaturated and partly unsaturated porous media. Quantitative Approaches in Systems Analysis No. 20, DLO Research Institute for Agrobiology and Soil Fertility and the C.T. de Wit Graduate School for Production Ecology, Wageningen, The Netherlands, 140 p.

Press W.H., B.P. Flannery, S.A. Teukolsky and W.T. Vetterling, 1992. Numerical recipes in Fortran 77. Second edition. The art of scientific computing. Cambridge University Press, Cambridge.

3 Cylindrical coordinates: FUSSIMR

Peter de Willigen and Marius Heinen

In this chapter we describe how water movement in cylindrical coordinates is implemented in the code FUSSIMR. We use the same notation convention as in Heinen and de Willigen (1998).

3.1 Discretization in cylindrical coordinates.

The equivalent of Richard's equation (multiplied by r for convenience) in cylindrical coordinates reads

$$r\frac{\partial \boldsymbol{q}}{\partial t} = -\frac{\partial}{\partial r}rq_r - \frac{\partial}{\partial \boldsymbol{y}}q_{\boldsymbol{y}} - \frac{\partial}{\partial z}rq_z - rS_w \qquad (3\text{-}1)$$

where

r	the radial coordinate	L
$\boldsymbol{y}$	the tangential coordinate	L
z	the vertical coordinate	L
$\boldsymbol{q}$	volumetric water content	L^3L^{-3}
t	time	T
q	water flux density $L^3L^{-2}T^{-1}$	
S_w	sink strength for water	$L^3L^{-3}T^{-1}$

The Darcy fluxes in cylindrical coordinates ($r,z,\boldsymbol{y}$) read

$$q_r = -K_r\frac{\partial h}{\partial r}, \quad q_z = -K_z\frac{\partial h}{\partial z} + K_z, \quad q_{\boldsymbol{y}} = -\frac{K_{\boldsymbol{y}}}{r}\frac{\partial h}{\partial \boldsymbol{y}} \qquad (3\text{-}2)$$

where

K	hydraulic conductivity	LT^{-1}
h	pressure head	L

In order to discretize this equation we integrate it over the control volume. The grid point in the control volume is indicated by the subscript P, its neighbors in the r-direction are indicated by the indexes W(est) and E(ast), in the $\boldsymbol{y}$-direction by L(eft) and R(ight) and in the z-direction by S(outh) and N(orth). The interfaces between the control volumes are indicated by lower case indexes, e.g. n denotes the interface between control volume P and N.

The integration of the **first term** of the right hand side of Eq. (3-1) yields

$$\int_{y_l}^{y_r}\int_{z_s}^{z_n}\int_{t}^{t+\Delta t}\int_{r_w}^{r_e}-\frac{\partial}{\partial r}rq_r\,drdtdzdy = \int_{y_l}^{y_r}\int_{z_s}^{z_n}-[rq_r]_{r_w}^{r_e}\,\Delta tdzdy = -[r_eq_{r,e}-r_wq_{r,w}]\Delta y\Delta z\Delta t \qquad (3\text{-}3)$$

The fluxes $q_{r,e}$ and $q_{r,w}$ are approximated by

$$q_{r,e}=-K_{r,e}\frac{h_E-h_P}{dr_e}, \quad q_{r,w}=-K_{r,w}\frac{h_P-h_W}{dr_w} \qquad (3\text{-}4)$$

Substitution of Eq. (3-4) in Eq. (3-3) yields

$$\int_{y_l}^{y_r}\int_{z_s}^{z_n}\int_{t}^{t+\Delta t}\int_{r_w}^{r_e}-\frac{\partial}{\partial r}rq_r\,drdtdzdy = \left[r_e\frac{K_{r,e}(h_E-h_P)}{dr_e}-r_w\frac{K_{r,w}(h_P-h_W)}{dr_w}\right]\Delta y\Delta z\Delta t \qquad (3\text{-}5)$$

Likewise the integration of the **second term** of the right hand side of Eq. (3-1) yields

$$\int_{r_w}^{r_e}\int_{z_s}^{z_n}\int_{t}^{t+\Delta t}\int_{y_l}^{y_r}-\frac{\partial}{\partial y}q_y\,dydtdzdr = \int_{r_w}^{r_e}\int_{z_s}^{z_n}-[q_y]_{y_l}^{y_r}\Delta tdzdr = -[q_{y,r}-q_{y,l}]\Delta r\Delta z\Delta t \qquad (3\text{-}6)$$

The fluxes $q_{y,l}$ and $q_{y,r}$ are approximated by

$$q_{y,r}=-\frac{K_{y,r}}{r_r}\frac{h_R-h_P}{dy_r}, \quad q_{y,l}=-\frac{K_{y,l}}{r_l}\frac{h_P-h_L}{dy_l} \qquad (3\text{-}7)$$

Substitution of Eq. (3-7) in Eq. (3-6) yields

$$\int_{r_w}^{r_e}\int_{z_s}^{z_n}\int_{t}^{t+\Delta t}\int_{y_l}^{y_r}-\frac{\partial}{\partial y}q_y\,dydtdzdr = -\left[\frac{K_{y,r}(h_R-h_P)}{r_rdy_r}-\frac{K_{y,l}(h_P-h_L)}{r_ldy_l}\right]\Delta r\Delta z\Delta t \qquad (3\text{-}8)$$

Note that $r_r = r_l$.

Integration of the **third term** of the right hand side of Eq. (3-1) eventually leads to

$$\int_{y_l}^{y_r}\int_{r_w}^{r_e}\int_{t}^{t+\Delta t}\int_{z_s}^{z_n}-\frac{\partial}{\partial z}rq_z\,dzdtdrdy = \int_{y_l}^{y_r}\int_{r_w}^{r_e}-r[q_r]_{z_s}^{z_n}\Delta tdrdy = -\left(q_{z,n}-q_{z,s}\right)\int_{r_w}^{r_e}rdr\Delta y\Delta t\Delta z$$

$$= -\left(q_{z,n}-q_{z,s}\right)\frac{r_e^2-r_w^2}{2}\Delta y\Delta t\Delta z \qquad (3\text{-}9)$$

The fluxes $q_{z,n}$ and $q_{z,s}$ are approximated by

$$q_{z,n} = -K_{z,n}\frac{h_N - h_P}{dz_n} + K_{z,n}, \quad q_{z,n} = -K_{z,s}\frac{h_P - h_S}{dz_s} + K_{z,s} \tag{3-10}$$

Substitution of Eq. (3-10) in Eq. (3-9) yields

$$\int_{y_l}^{y_r}\int_{r_w}^{r_e}\int_{t}^{t+\Delta t}\int_{z_s}^{z_n} -\frac{\partial}{\partial z}rq_z\,\mathrm{d}z\mathrm{d}t\mathrm{d}r\mathrm{d}y =$$

$$\left[\frac{r_e^2 - r_w^2}{2}\left(K_{z,n}\frac{h_N - h_P}{dz_n} - K_{z,s}\frac{h_P - h_S}{dz_s}\right) + \frac{r_e^2 - r_w^2}{2}\left(K_{z,n} - K_{z,s}\right)\right]\Delta y\Delta t\Delta z \tag{3-11}$$

Integration of the **source term** of the right hand side of Eq. (3-1) finally yields

$$-S_P\Delta V\Delta t \tag{3-12}$$

where DV is the volume of the control volume given by

$$\Delta V = \frac{r_e^2 - r_w^2}{2}\Delta y\Delta z \tag{3-13}$$

Integration of the **storage term** (the left hand side) of Eq. (3-1) yields

$$\left[q_P - q_P^0\right]\Delta V \tag{3-14}$$

but as before by using a truncated Taylor expansion around h_p^n it is replaced by

$$\left[C_P^n\left(h_P^{n+1} - h_P^n\right) + \left(q_P^n - q_P^0\right)\right]\Delta V_P \tag{3-15}$$

where
$\quad C \qquad$ differential moisture capacity $\qquad\qquad\qquad\qquad$ L^{-1}

Combining and rearranging one gets the **discretized equivalent** of Eq. (3-1)

$$Ah_P^{n+1} = A_W h_W^{n+1} + A_E h_E^{n+1} + A_N h_N^{n+1} + A_S h_S^{n+1} + A_L h_L^{n+1} + A_R h_R^{n+1} + b \tag{3-16}$$

with

$$A_R = \frac{K_{y,r}\Delta r\Delta z}{r_r dy_r} \tag{3-17}$$

$$A_L = \frac{K_{y,l} \Delta r \Delta z}{r_l \boldsymbol{d}\boldsymbol{y}_l} \tag{3-18}$$

$$A_E = \frac{K_{r,e} r_e \Delta \boldsymbol{y} \Delta z}{\boldsymbol{d}r_e} \tag{3-19}$$

$$A_W = \frac{K_{r,w} r_w \Delta \boldsymbol{y} \Delta z}{\boldsymbol{d}r_w} \tag{3-20}$$

$$A_N = \frac{K_{z,n} \Delta \boldsymbol{y}}{\boldsymbol{d}z_n} \frac{r_e^2 - r_w^2}{2} \tag{3-21}$$

$$A_S = \frac{K_{z,s} \Delta \boldsymbol{y}}{\boldsymbol{d}z_s} \frac{r_e^2 - r_w^2}{2} \tag{3-22}$$

$$b = A_P^0 h_P^0 - \left(\boldsymbol{q}_P^{\boldsymbol{n}} - \boldsymbol{q}_P^0\right)\frac{\Delta V_P}{\Delta t} - \left(K_{z,n} - K_{z,s}\right)\frac{r_e^2 - r_w^2}{2}\Delta \boldsymbol{y} - S_P \Delta V_P \tag{3-23}$$

$$A_P^0 = C_P^{\boldsymbol{n}} \frac{\Delta V_P}{\Delta t} \tag{3-24}$$

$$A = A_W + A_E + A_N + A_S + A_L + A_R + A_P^0 \tag{3-25}$$

3.2 FUSSIMR in two dimensions

The code FUSSIMR is at present only available for two-dimensional *r-z* situations, i.e. no gradients in the tangential direction exist. The above equations remain valid; only the equations simplify and some coefficients vanish. In case of transport in radial (*r*) and vertical (*z*) direction only the coefficients A_L and A_R vanish and $\Delta \boldsymbol{y}$ should be replaced by 2π..

For completeness, in case of transport in radial (*r*) and tangential (*y*) direction the coefficients A_N and A_S vanish, while Δz should be replaced by 1.

3.3 Boundary conditions

3.3.1 In r-direction

3.3.1.1 The outer radial boundary of the cylinder

Prescribed flux
The first term at the RHS of Eq. (3-3) be formulated as

$$\int\limits_{\boldsymbol{y}_l}^{\boldsymbol{y}_r}\int\limits_{z_s}^{z_n}\int\limits_{t}^{t+\Delta t}\int\limits_{r_w}^{r_e}-\frac{\partial}{\partial r}rq_r\,\mathrm{d}r\mathrm{d}t\mathrm{d}z\mathrm{d}\boldsymbol{y}=\int\limits_{\boldsymbol{y}_l}^{\boldsymbol{y}_r}\int\limits_{z_s}^{z_n}-\left[rq_r\right]_{r_w}^{r_e}\Delta t\mathrm{d}z\mathrm{d}\boldsymbol{y}$$

$$=\left[-r_e q_{r,e}-\frac{K_{r,w}r_w\left(h_P-h_W\right)}{dr_w}\right]\Delta\boldsymbol{y}\Delta z\Delta t \tag{3-26}$$

The flux $q_{r,e}$ is the prescribed flux over the outer radial surface and $r_e\Delta\boldsymbol{y}\Delta z$ is the outer surface of the control volume, so the product of both is the volumetric flux out or into the control volume. So the discretized equation for the boundary control volumes is similar to Eq. (3-16), except that now $A_E = 0$, and the term $r_e\Delta\boldsymbol{y}\Delta zq_{r,e}$, after division by Δt, should be added to b.

Prescribed pressure head
The easiest way to handle this condition is to make all the coefficients, A_E, A_w, A_N, A_S, A_B, A_T zero and substitute $A = 1$, and $b = h_{r1}$ where h_{r1} is the prescribed pressure head. But as explained earlier this leads to difficulties with one of the solution methods used. So again the following procedure was followed: the normal discretization equation Eq. (3-16) is used, but A and b are now given as

$$A = Q \tag{3-27}$$

and

$$b = h_{r_1} Q \tag{3-28}$$

where Q is a number so large that the other terms are insignificant, this yields the desired result.

3.3.1.2 The inner radial boundary of the cylinder

At the inner boundary - the longitudinal axis -, the condition is always that of zero-flux, so here

$$A_W = 0 \tag{3-29}$$

the other terms being similar to those given before. If a hollow cylinder is considered, the inner boundary can be of the same type as the outer boundary as described in the previous sub-section.

3.3.2 In z-direction

The handling of boundary conditions at $z = 0$ and $z = z_1$ is similar to that for the radial boundary conditions. For prescribed flux at the top $A_N = 0$, and to b a term $0.5(r_e^2 - r_w^2)\Delta y q_{z,n}$ is added; at the bottom one sets $A_S = 0$, and adds $0.5(r_e^2 - r_w^2)\Delta y q_{zs}$ to b. The boundary condition of prescribed pressure head is dealt with by setting as before: $A = Q$ (Eq. (3-27)) and $b = h_{r1}Q$ (Eq. (3-28)).

3.4 Geometry

The soil cylinder with radius R_1 is divided in NR rings and NL layers (and $NPSI$ segments). The radial coordinate of the grid points is located midway between the boundaries of the control volumes. The first grid point lies in the center of the soil cylinder ($r = 0$). For the outer control volume the grid point lies at the outer boundary ($r = R_1$). In a (r,z) two-dimensional system the state variables pertain to gridlines (circles) rather than to grid points.

In FUSSIMR the following variables are used:
R(I)   coordinate of the radial outer boundary of CV I
RGRID(I)   coordinate of grid point I
DR(I)   radial thickness of CV I
DISTR(I)   radial distance between grid point I and I+1

At this time there are two options to divide the soil cylinder in NR rings. First, the user can enter the thickness of each ring. Secondly, the user can enter the radius R_1 of the cylinder and the number of rings NR. Then, the thickness of the rings are computed such that the volumes of each of the control volumes are the same. In that case

$$\boldsymbol{p}r_1^2 = \boldsymbol{p}\left(r_2^2 - r_1^2\right) = \boldsymbol{p}\left(r_3^2 - r_2^2\right) = \ldots = \boldsymbol{p}\left(r_{NR}^2 - r_{NR-1}^2\right) \tag{3-30}$$

From this it follows that

$$r_i = r_1\sqrt{i} \tag{3-31}$$

and so

$$r_1\sqrt{NR} = R_1 \tag{3-32}$$

or

$$r_1 = \frac{R_1}{\sqrt{NR}} \tag{3-33}$$

Now all r_i can be computed. Furthermore, any DR(I) can be computed as

$$DR(I) = r_1\left(\sqrt{I} - \sqrt{I-1}\right) \tag{3-34}$$

The sum of all DR(I) equals R_1.

Surface areas
In computations of flux densities the surface areas perpendicular to the direction of water movement are needed if volume fluxes ($cm^3 d^{-1}$) are required, e.g. to compute amount of water that passed a certain boundary. In rectangular coordinates these surface areas are simply $\Delta x \Delta y = \Delta x.1 = \Delta x$ or $\Delta z \Delta y = \Delta z.1 = \Delta z$. In cylindrical coordinates, however, we have:
for flow in z direction (assuming only flow in (r,z) domain, i.e. no y dimensioning)
　　SURFZ(I) = p (R(I)^2 - R(I-1)^2) = p DR(I) (R(I) + R(I-1))
for flow in r direction (assuming only flow in (r,z) domain, i.e. no y dimensioning)
　　SURFR(I,J) = 2p R(I) DZ(J)

3.5　　Verification

A transient (r,z) analytical solution for heat transfer in a finite cylinder with unit initial temperature, zero surface temperature and constant conductivity is used to verify the numerical simulation model. The cylinder is represented by $-Z/2 < z < Z/2$, $0 < r < R_1$. The analytical solution is given by Carslaw and Jaeger (1959; their Eq. (5) on page 225)

$$u(r,z) = c(r,R_1)z(z,Z/2) \tag{3-35}$$

The two functions are given by (Carslaw and Jaeger, 1959; their Eq. (1) on page 225)

$$c(r, R_1) = \frac{2}{R_1}\sum_{n=1}^{\infty}\exp\left(-Ka_n^2 t\right)\frac{J_0(ra_n)}{a_n J_1(R_1 a_n)} \tag{3-36}$$

where a_n are the positive roots of

$$J_0(R_1 a) = 0 \tag{3-37}$$

and (Carslaw and Jaeger, 1959; their Eq. (6) on page 173)

$$z(z, Z/2) = \frac{4}{p}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)}\exp\left(-K\frac{(2n+1)^2 p^2}{4(Z/2)^2}t\right)\cos\left(\frac{(2n+1)pz}{2(Z/2)}\right) \tag{3-38}$$

respectively.

This verification is analogous to the verification in sections 6.1 and 6.3 of Heinen and de Willigen (1998), so we do not describe the details of how the simulation is carried out. The comparison between numerical and analytical solutions is very good for both water movement and solute transport (Figure 3-1).
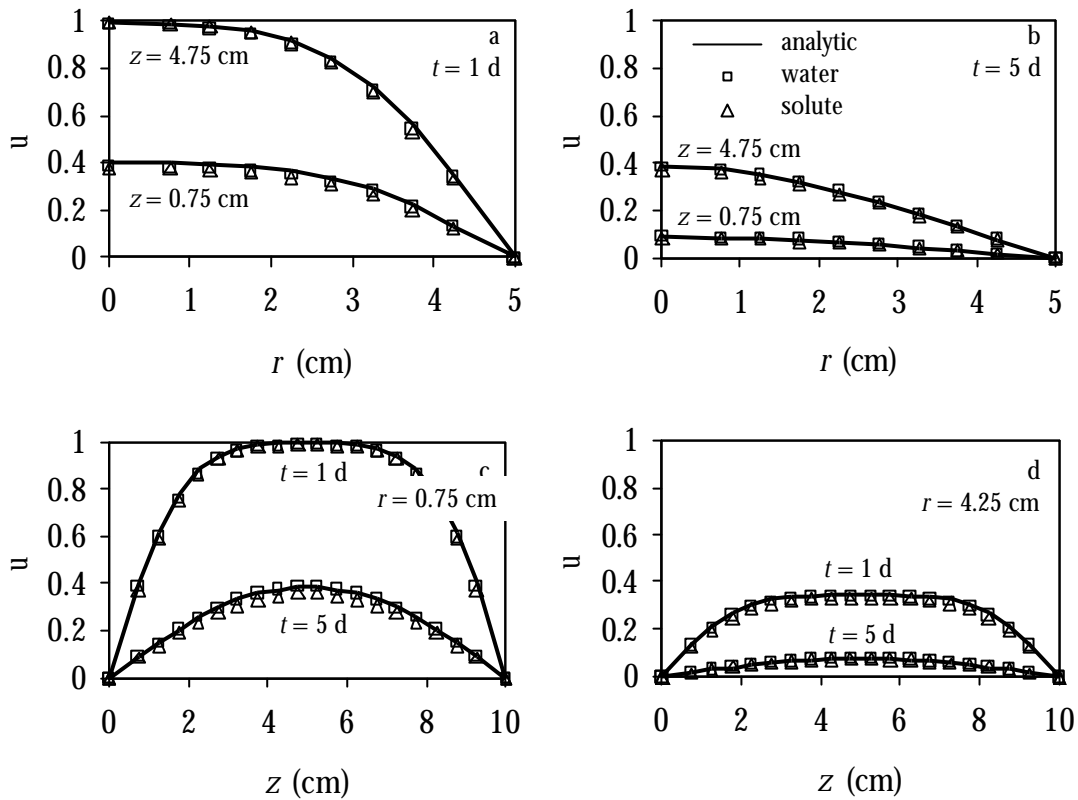
Figure 3-1. Comparison between numerical (symbols) and analytical (lines) solutions for both water movement (?) and solute (?) transport.

3.6 References

Carslaw H.S. and J.C. Jaeger. 1959. Conduction of heat in solids, 2nd ed. Macmillan, New York.

Heinen M. and P. de Willigen, 1998. FUSSIM2 A two-dimensional simulation model for water flow, solute transport and root water and root nutrient uptake in unsaturated and partly unsaturated porous media. Quantitative Approaches in Systems Analysis No. 20, DLO Research Institute for Agrobiology and Soil Fertility and the C.T. de Wit Graduate School for Production Ecology, Wageningen, The Netherlands, 140 p.

4 Extension to the van Genuchten-Mualem description of the hydraulic properties in FUSSIM2

Marius Heinen

4.1 Introduction

Movement of water through porous media is determined by the hydraulic properties of the porous media. The hydraulic properties are given by the water retention and hydraulic conductivity characteristics. These characteristics describe the relationships between pressure head h [L], volumetric water content q [L^3L^{-3}] and hydraulic conductivity K [LT^{-1}]. For soils, but also for coarse porous media used as root zone substrates in horticulture (e.g. Otten, 1994; Heinen, 1997), these relationships are commonly described by the van Genuchten (1980) $q(h)$ and Mualem (1976) $K(q)$ (or $K(h)$) relationships. These relationships are incorporated in the simulation model FUSSIM2 (Heinen and de Willigen, 1998).

For some soils, especially clayey soils, it appears that the description of $K(q)$ fails near saturation. Vogel and Cislerova (1988) proposed an extension of the van Genuchten-Mualem equations. These extensions have been included in the Hydrus_2D model of Simunek *et al.* (1994) and have been successfully used by de Vos (1997) for describing water flow and nutrient transport in layered silt loam soil.

It was decided to extend the van Genuchten-Mualem functions of the model FUSSIM2. This chapter describes the new functions, and discusses how these have been incorporated in FUSSIM2. Additionally, attention is paid to the matric flux potential as it is used in the water uptake module in FUSSIM2.

4.2 Theory

Vogel and Cislerova (1988) presented the following descriptions for $q(h)$ and $K(h)$ (Figure 4-1)

$$q(h) = \begin{cases} q_a + \dfrac{q_m - q_a}{\left(1 + |ah|^n\right)^m} & h < h_s \\ q_s & h \geq h_s \end{cases} \tag{4-1}$$

and

$$K(h) = \begin{cases} K_s K_r(h) & h \leq h_k \\ K_k + \dfrac{(h - h_k)(K_s - K_k)}{(h_s - h_k)} & h_k < h < h_s \\ K_s & h \geq h_s \end{cases} \tag{4-2}$$

respectively, where

$$K_r = \frac{K_k}{K_s} \left(\frac{S}{S_k} \right)^l \left[\frac{F(\boldsymbol{q}_r) - F(\boldsymbol{q})}{F(\boldsymbol{q}_r) - F(\boldsymbol{q}_k)} \right]^2 \tag{4-3}$$

$$F(\boldsymbol{q}) = \left[1 - \left(\frac{\boldsymbol{q} - \boldsymbol{q}_a}{\boldsymbol{q}_m - \boldsymbol{q}_a} \right)^{1/m} \right]^m \tag{4-4}$$

$$m = 1 - \frac{1}{n}, \quad n > 1 \tag{4-5}$$

$$S = \frac{\boldsymbol{q} - \boldsymbol{q}_r}{\boldsymbol{q}_s - \boldsymbol{q}_r} \tag{4-6}$$

$$S_k = \frac{\boldsymbol{q}_k - \boldsymbol{q}_r}{\boldsymbol{q}_s - \boldsymbol{q}_r} \tag{4-7}$$

in which

$\boldsymbol{q}_r$	residual water content	$L^3 L^{-3}$
$\boldsymbol{q}_s$	water content at saturation	$L^3 L^{-3}$
$\boldsymbol{q}_a$	(extrapolated) fictitious $\boldsymbol{q}_r$; $\boldsymbol{q}_a \leq \boldsymbol{q}_r$	$L^3 L^{-3}$
$\boldsymbol{q}_s$	(extrapolated) fictitious $\boldsymbol{q}_s$; $\boldsymbol{q}_m \geq \boldsymbol{q}_s$	$L^3 L^{-3}$
h	pressure head	L
h_s	air-entry value	L
h_k	pressure head above which $K(h)$ becomes linear	L
K_s	hydraulic conductivity at saturation	LT^{-1}
K_k	hydraulic conductivity at h_k	LT^{-1}
$\boldsymbol{a}$	curve shape parameter	L^{-1}
$n, m, \boldsymbol{l}$	curve shape parameters	-
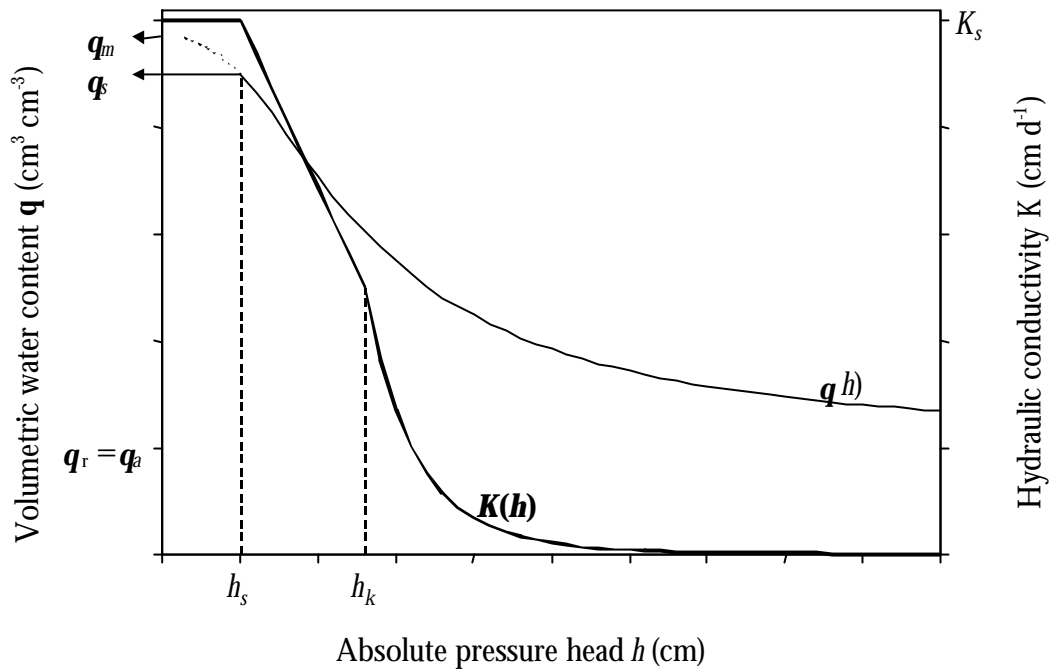
Figure 4-1. Schematic representation of the water retention characteristic $q(h)$ and the hydraulic conductivity characteristic K(h) as given by Eqs. (4-1) and (4-2), respectively. The following parameters were used: $q_a = q_r = 0.1$ cm³ cm⁻³, $q_s = 0.45$ cm³ cm⁻³, $a = 0.05$ cm⁻¹, n = 2.5, m = 0.6, $K_s = 50$ cm d⁻¹, $l = 0.5$, $K_k = 25$ cm d⁻¹, $h_k = -26$ cm, $h_s = -10$ cm, $q_m = 0.486$ cm³ cm⁻³ (computed from Eq. (4-1) with $q = q_s$, h = h_s), and $q_k = 0.303$ cm³ cm⁻³ (computed from Eq. (4-1) with h = h_k).

So far, in FUSSIM2 the air-entry value is not considered, i.e. $h_s = 0$. In that case we have $q_a = q_r$ and $q_m = q_s$. Eqs. (4-1)-(4-4) are then written as (note: $F(q_r) = 1$)

$$q(h) = \begin{cases} q_r + \dfrac{q_m - q_r}{\left(1 + |ah|^n\right)^m} & h < 0 \\ q_s & h \geq 0 \end{cases} \tag{4-8}$$

$$K(h) = \begin{cases} K_s K_r(h) & h \leq h_k \\ K_k - \dfrac{(h - h_k)(K_s - K_k)}{h_k} & h_k < h < 0 \\ K_s & h \geq 0 \end{cases} \tag{4-9}$$

$$K_r = \frac{K_k}{K_s}\left(\frac{S}{S_k}\right)^l \left[\frac{1 - F(q)}{1 - F(q_k)}\right]^2 \tag{4-10}$$

$$F(q) = \left[1 - \left(\frac{q - q_r}{q_s - q_r}\right)^{1/m}\right]^m = \left[1 - S^{1/m}\right]^m \tag{4-11}$$

respectively. Now, Eq. (4-8) is no longer different from the expression already used in FUSSIM2. Only the description of K is different. In FUSSIM2 there are two functions that can compute K: one based on known q ($K(q)$) and the other based on known h ($K(h)$). The first is used for solving the water flow problem, and has the advantage of not being influenced by hysteresis, the second is used in solving the water uptake model (in which hysteresis is not considered). Equation (4-9) expresses K as a function of both q and h. Since q and h are related through Eq. (4-8) (disregarding hysteresis), it is possible the substitute either h or q in Eq. (4-9) to obtain $K(q)$ and $K(h)$, respectively. The $K(q)$ relationship reads

$$K(q) = \begin{cases} K_k \left(\dfrac{S}{S_k}\right)^l \left[\dfrac{1-F(q)}{1-F(q_k)}\right]^2 & q \leq q_k \\[3mm] K_k + \left(1 - \dfrac{G(q)}{G(q_k)}\right)(K_s - K_k) & q_k < q < q_s \\[3mm] K_s & q = q_s \end{cases} \tag{4-12}$$

with

$$G(q) = -\frac{1}{a}\left(S^{-1/m} - 1\right)^{1/n} \tag{4-13}$$

$$G(q_k) = -\frac{1}{a}\left(S_k^{-1/m} - 1\right)^{1/n} \tag{4-14}$$

and the $K(h)$ relationship reads (after some algebraic rearrangement)

$$K(h) = \begin{cases} K_k C_k \dfrac{\left(\left(1+|ah|^n\right)^m - |ah|^{n-1}\right)^2}{\left(1+|ah|^n\right)^{m(l+2)}} & h \leq h_k \\[3mm] K_k - \dfrac{(h-h_k)(K_s - K_k)}{h_k} & h_k < h < 0 \\[3mm] K_s & h \geq 0 \end{cases} \tag{4-15}$$

where

$$C_k = \frac{\left(1+|ah_k|^n\right)^{m(l+2)}}{\left(\left(1+|ah_k|^n\right)^m - |ah_k|^{n-1}\right)^2} \tag{4-16}$$

For the case where one does not want to consider a linear part in the K curve near saturation, we have (require) $K_k = K_s$, $h_k = 0$ and $\boldsymbol{q}_k = \boldsymbol{q}_s$. In that case Eqs. (4-12) and (4-15) reduce to (note: $S_k = 1$, $F(\boldsymbol{q}_k) = 0$, $C_k = 0$)

$$K(\boldsymbol{q}) = \begin{cases} K_s S^l \left(1 - \left(1 - S^{1/m}\right)^m\right)^2 & \boldsymbol{q} \le \boldsymbol{q}_s \\ K_s & \boldsymbol{q} = \boldsymbol{q}_s \end{cases} \tag{4-17}$$

and

$$K(h) = \begin{cases} K_s \dfrac{\left(\left(1 + |\boldsymbol{a}h|^n\right)^m - |\boldsymbol{a}h|^{n-1}\right)^2}{\left(1 + |\boldsymbol{a}h|^n\right)^{m(l+2)}} & h \le 0 \\ K_s & h \ge 0 \end{cases} \tag{4-18}$$

respectively. Equations (4-17) and (4-18) are the ones that were originally used in FUSSIM2 (Heinen and de Willigen, 1998; their Eqs. [184] and [187], respectively).

In Eqs. (4-13) and (4-14) the $\boldsymbol{a}$-parameter appears. For hysteretic cases, the model FUSSIM2 assumes that for drying and wetting different $\boldsymbol{a}$ values have to be used. Fortunately, in Eq. (4-12) Eq. (4-13) is divided by Eq. (4-14), so that the $\boldsymbol{a}$-parameter disappears.

4.3   Matric Flux potential

In the transpiration module of FUSSIM2 the matric flux potential is needed (see description of this module in Heinen and de Willigen, 1998). The matric flux potential represents the integral of the $K(h)$ relationship and is given as

$$\boldsymbol{f} = \int_{h_L}^{h_H} K(h)\mathrm{d}h \tag{4-19}$$

in which

$\boldsymbol{f}$	matric flux potential (< 0)	$L^2 T^{-1}$
h_H	higher integration limit	L
h_L	lower integration limit	L

In FUSSIM2 there is a subroutine (MFLP(D)) that computes $\boldsymbol{f}$. Here the absolute pressure head is used, denoted as P, with $P = -h$. Furthermore, we are only interested in the unsaturated zone, so that we have to consider only the first two expressions in the $K(h)$ relationship (Eq. (4-15)). Combining Eqs. (4-19) and (4-15) thus yields

$$
\boldsymbol{f} = \begin{cases} K_k C_k \displaystyle\int_{P_L}^{P_H} \left(\dfrac{\left(\left(1+(aP)^n\right)^m - (aP)^{n-1} \right)^2}{\left(1+(aP)^n\right)^{m(I+2)}} \right) \mathrm{d}P & P \geq P_k \\[4mm] \displaystyle\int_{P_L}^{P_H} \left(K_k + \dfrac{(P_k - P)(K_s - K_k)}{P_k} \right) \mathrm{d}P & 0 < P < P_k \end{cases}
\tag{4-20}
$$

For $P_k = 0$ (no linear part in K curve) we require $K_k = K_s$ and $h_k = 0$, in which case Eq. (4-20) reduces to

$$
\boldsymbol{f} = K_s \int_{P_L}^{P_H} \left(\dfrac{\left(\left(1+(aP)^n\right)^m - (aP)^{n-1} \right)^2}{\left(1+(aP)^n\right)^{m(I+2)}} \right) \mathrm{d}P
\tag{4-21}
$$

Equation (4-21) is also obtained when the first term of Eq. (4-18) is substituted in Eq. (4-19).

We have to consider the following four cases (note: $P_L < P_H$).

1. Both P_L and P_H are less than P_k so that we have to consider the linear part of $K(h)$. The matric flux potential is given by the second term of Eq. (4-20) and is given as

$$
\boldsymbol{f} = K_s (P_H - P_L) - \dfrac{(K_s - K_k)}{2 P_k} \left(P_H^2 - P_L^2 \right)
\tag{4-22}
$$

2. Both P_L and P_H are larger than P_k so that we have to consider the first term in Eq. (4-20). In FUSSIM2 the integral in Eq. (4-21) is solved numerically. We can still use this solution and multiply this result with $K_k C_k$ (instead of multiplying it with K_s).

3. When P_L is less than P_k and P_H is larger than P_k, the matric flux potential is the sum of both integrals in Eq. (4-20) with proper integral limits. For the linear part (between P_L and P_k) the result follows from Eq. (4-22) (substituting P_H by P_k)

$$
\boldsymbol{f} = K_s (P_k - P_L) - \dfrac{(K_s - K_k)}{2 P_k} \left(P_k^2 - P_L^2 \right)
\tag{4-23}
$$

4. When $P_k = 0$, i.e. we do not consider a linear part in the K curve, the old solution as used in FUSSIM2, i.e. the solution of Eq. (4-21) remains valid.

4.4   Implementation in FUSSIM2

The functions COND, CONDD, CONDW and CONDWD have been changed so that they compute $K(h)$ according to Eq. (4-15) (single precision in COND, double precision in CONDD) and $K(q)$ according to Eq. (4-12) (single precision in CONDW, double precision in CONDWD). These computations require additional parameters, i.e. K_k and q_k or h_k. It was decided that the user should supply both K_k and q_k, and when necessary h_k can be computed using the function PRES(D) (with the a-parameter for the drying curve). The common block /VGEN/ is extended with these two additional parameters. The routine GTSOIL is adapted such that the two new variables are read from the soils database file. The model TRANSP required some additional changes in order to take care for correct transfer of parameters to several internal subroutines or functions (through common blocks /FFP1/ and /FUNKH/, and in argument lists of COMAS and ESTDPH).

After reading the parameters (using GTSOIL) it is checked whether K_k and q_k have good values. In case $q_k > q_s$ or $q_k \beta q_r$ we set $q_k = q_s$ and $K_k = K_s$, in this way FUSSIM2 will not consider a linear part in the K curve. Similarly, In case $K_k > K_s$ or $K_k \beta 0$ we set $K_k = K_s$ and $q_k = q_s$. Other checks are not possible. It is assumed that the user is well familiar with the extended van Genuchten-Mualem model, so that the user supplies realistic values for K_k and q_k.

The functions MFLP (single precision) and MFLPD (double precision) have been changed according to Eqs. (4-20)-(4-23).

In FUSSIM2 evaporation reduction is computed using available data from an input file (typically with extension .EXT). This EXT-file is constructed with the program EXTMAKE. In this program the functions CONDWD, CONDD and MFLPD are used. EXTMAKE has been adapted such that proper argument lists in the calls to these functions are used.

A simple program is made to transform the old SOILS.DB file into a new SOILS.DB in which the two variables K_k and q_k are added. The values for these two variables are $K_k = K_s$ and $q_k = q_s$. The name of this program is CHANGEDB.

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5 From potential to actual evaporation of water at the soil surface

Marius Heinen and Peter de Willigen

5.1 Introduction

Water vapor deficit in the atmosphere induces an evaporative demand from the soil and the crop. There are several methods to compute the potential evapotranspiration ET_p (LT^{-1}) demand, e.g. the Penman-Monteith equation. There are also ways to divide ET_p into potential transpiration by the crop T_p (LT^{-1}) and potential evaporation of water from the soil surface E_p (LT^{-1}), e.g. via the leaf area index. Evaporation of water at the soil surface occurs through water transport across the soil-atmosphere interface and through the vapor phase. Considering evaporation at the soil surface would mean to consider vapor transport as well in a simulation model, such as FUSSIM2 (Heinen and de Willigen, 1998). In this chapter we have chosen to adopt an empirical approach to consider evaporation at the soil surface using data from the literature. This chapter describes the implementation of this method in FUSSIM2.

It is assumed that E_p is known at each time (see above). Based on the soil condition near the surface it is checked if E_p can be reached, or if not, what the actual evaporation of water at the soil surface E_a is. Van Keulen (1975) and van Keulen and Seligman (1987) presented an empirical relationship between the ratio E_a/E_p and the pressure head near the soil surface h_0 (L), i.c. at $z_0 = 1$ cm below the soil surface (Figure 5-1). This relationship was obtained from their simulation model, in which they used a 2 cm thick top layer. In general, in FUSSIM2 the node of the first layer lies at the soil surface, i.e. $z = 0$ cm. The node of the second layer lies in the middle of the second layer. Since the thickness of the layers may be variable, we do not know the pressure head at 1 cm depth. Next we will explain how h_0 is obtained. The only restriction is that the node of the second layer lies deeper than 1 cm. Furthermore, we assume only vertical movement of water near the surface.
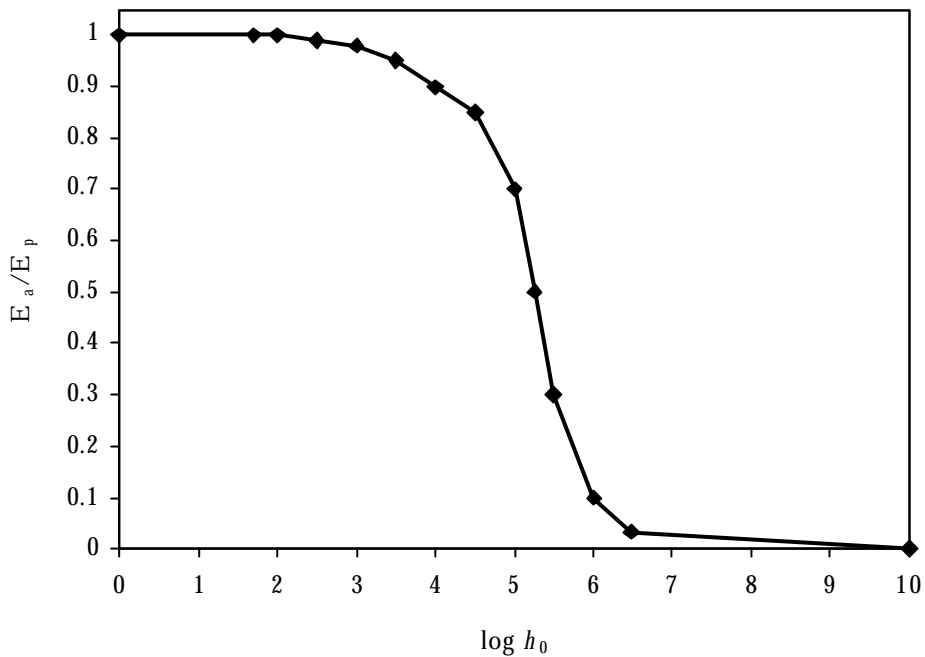
Figure 5-1. The relationship $E_a/E_p(h_0)$ according to van Keulen (1975) and van Keulen and Seligman (1987).

In general the simulation model knows the pressure head at some depth z_1 ($z_1 > z_0$) close to the soil surface, denoted by h_1. When the soil dries out, there is no linear drop in h near the surface, due to the highly non-linear hydraulic properties of the soil. We make use of a steady state approach. At steady state there is a constant flux density between z_1 and z_0 which equals the evaporation E (< 0). According to Darcy's law we have

$$E = -K \frac{\partial h}{\partial z} + K \tag{5-1}$$

where

E	evaporation rate	LT^{-1}
K	hydraulic conductivity (being a function of h)	LT^{-1}
h	pressure head	L
z	vertical coordinate	L

Since h is only dependent on z and no longer on time, we may replace the partial derivatives in Eq. (5-1) by normal derivatives to yield

$$\frac{K}{K-E} \frac{\mathrm{d}h}{\mathrm{d}z} = 1 \tag{5-2}$$

Integrating Eq. (5-2) from $z = z_1$, $h = h_1$ to $z = z_0$, $h = h_0$ gives

$$\int_{h_1}^{h_0} \frac{K}{K - E}\,\mathrm{d}h = \int_{z_1}^{z_0} 1\,\mathrm{d}h = z_0 - z_1 \tag{5-3}$$

For a known $K(h)$ relationship the left hand side of Eq. (5-3) can be computed to give the steady state solution $z(h)$. For known z_0, z_1 and h_1, the unknown h_0 can then be computed. In FUSSIM2 the $K(h)$ relationship of Mualem (1976) is used (see chapter 4). Since we do not know the integral of this relationship, Eq. (5-3) cannot be solved analytically. It is estimated by using the Romberg integration method (Press *et al.*, 1992). Since E is a function of h_0 (Figure 5-1), the solution of Eq. (5-3) is obtained iteratively. For K we use $K(h_0)$. The solution procedure is described in the Appendix at the end of this chapter.

The integration routine takes much computational time, especially when the soil becomes drier. For this reason, and the fact that this procedure is an empirical one, we have decided not to implement the computation in the simulation model FUSSIM2 during the dynamic session of the computations. Instead, we make use of pre-made two-way tables during initialization. For a given soil type and a given position z_1, a table file is constructed during initialization. For several values of E_p and several values of h_1 the values of h_0 are computed. The program FUSSIM2 then searches in this table the four entries of this two-way table (the two nearest E_p and the two nearest h_1 values), and the estimate for h_0 is obtained through linear interpolation. The corresponding required E_a then simply follows from Figure 5-1.

5.2 Example

As an illustration of evaporation reduction we give an example of a clay soil column that is exposed to an evaporative demand E_p of 1 cm/d. Initially, h inside the 50 cm long column is in equilibrium with h at the bottom equal to –1000 cm. Already after the first day we see that the actual evaporation is smaller than the potential evaporation, and this difference increases in time (Figure 5-2). The corresponding changes in water content profile are given in Figure 5-3.
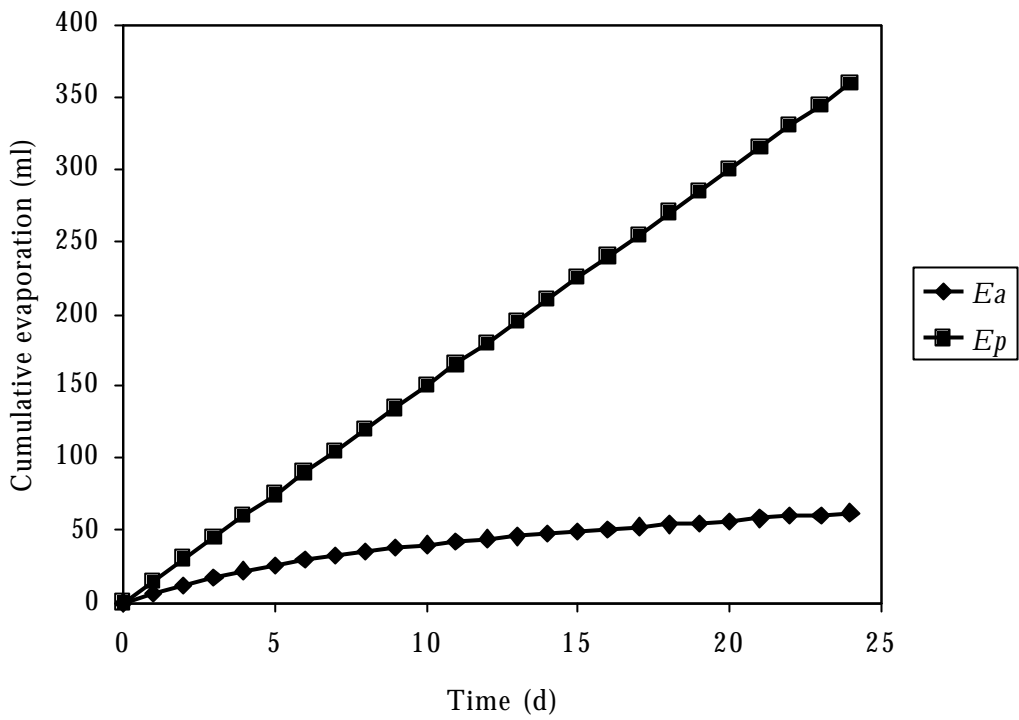
Figure 5-2. Cumulative potential evaporation and simulated cumulative actual evaporation at the soil surface.
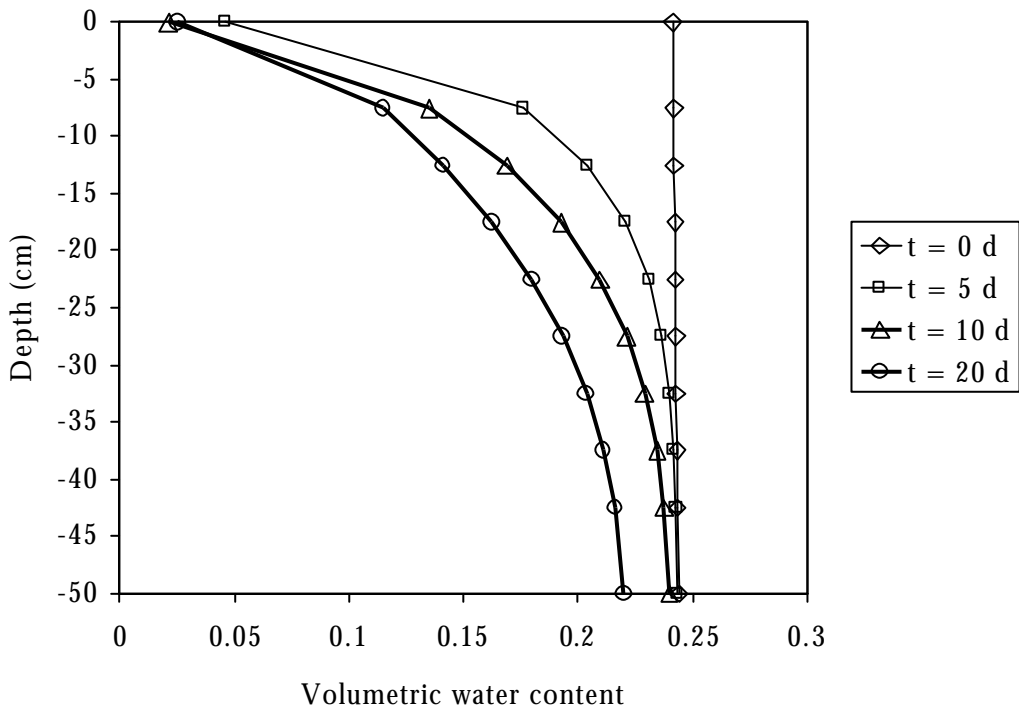
Figure 5-3. Simulated volumetric water content − depth profiles at several times during evaporation.

5.3 References

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5.4 Appendix

Step 1
Find two estimates for h_0, one for which the left hand side (LHS) of Eq. (5-3) is larger than z_0-z_1 and one for which the LHS is smaller than z_0-z_1.

Step 1.1
The initial estimate for h_0 comes from Eq. (5-2) by assuming $\mathrm{d}h = h_0$-h_1 and $\mathrm{d}z = z_0$-z_1

$$h_0 = h_1 + \frac{K - E}{K}(z_0 - z_1) \tag{5-5}$$

Step 1.2
The estimate of h_0 obtained in step 1.1 is either to high or too low. Using a bracketing method (Press *et al.*, 1992) a second estimate of h_0 is obtained which is too low or too high, respectively.

Step 2
In the interval of the two estimates of h_0 as obtained in Step 1, the true value of h_0 is found by means of the method of false position (Press *et al.*, 1992).

In all steps and computations E is adapted based on the current estimate of h_0 according to Figure 5-1. The data points in Figure 5-1 are stored in a table, and for intermediate values of h_0 the reduction value is obtained through linear interpolation.

6 Infiltration and runoff of water at the soil surface

Marius Heinen and Peter de Willigen

6.1 Introduction

Infiltration of water at the soil surface is generally modeled as a flux density boundary condition in simulation models. However, such flux boundary conditions may be ill-posed. That is, it may be possible that the physically maximum possible infiltration rate, as determined by the soil physical status at the soil surface, is less than the rainfall or irrigation rate. In that case, only the maximum possible rate will be achieved, and the water that does not enter the soil is left behind, known as ponding. On sloping surfaces, this ponded water will move down slope (overland flow). When (part) of this amount leaves the surface of interest it is called runoff. Here we describe the treatment of water infiltration, ponding, overland flow and runoff as implemented in FUSSIM2.

6.2 Overland flow and maximum infiltration rate

We start with describing the process of overland flow, which will give us an equation to describe runoff on sloping soil surfaces. For the case of non-sloping surfaces, this equation relates to ponding. We have chosen the approach of Hillel and Hornberger (1979) and Hillel (1980).

The basic equation governing the rate of flow in a channel, here applied to overland flow, is given as

$$Q = VA \tag{6-1}$$

where Q is the flow rate, V is the average velocity, and A is the cross-sectional area of flow. The governing conservation of matter (continuity) equation requires that the change of water level y with time t is equal to the negative change of flow rate with distance x corrected for the net change due to rainfall r and infiltration I

$$\frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = r - i \tag{6-2}$$

Considering forces and shear stresses acting on the flowing water along the sloping face it can be determined that V is related to y and the slope $\boldsymbol{a}$ according to

$$V = C y^{1/2} \boldsymbol{a}^{1/2} \tag{6-3}$$

where C is known as the Chezy coefficient. Experimentally it has been observed that C is not constant, but depends on y and the surface roughness n as follows

$$C = \frac{y^{1/6}}{n} \tag{6-4}$$

Combining Eqs. (6-3) and (6-4) yields the Manning's equation

$$V = \frac{y^{2/3} \boldsymbol{a}^{1/2}}{n} \tag{6-5}$$

Multiplying by y gives the discharge per unit width

$$Q = \frac{y^{5/3} \boldsymbol{a}^{1/2}}{n} \approx \frac{y^2 \boldsymbol{a}^{1/2}}{n} \tag{6-6}$$

In practice, the power 2 in Eq. (6-6), rather than the power 5/3, gave satisfactorily results for overland flow, which will be adopted here as well. The surface roughness n has been tabulated in the literature (e.g. Sellin, 1969). It ranges between 0.001 for extremely smooth channels to 0.1 for flood plains with a growth of heavy timber. For bare soil surfaces or soil surfaces with a cover of short grass, a value of $n = 0.03$ seems to be reasonable.

Combining Eqs. (6-2) and (6-6) yields the following kinematic wave equation

$$\frac{\partial y}{\partial t} + \boldsymbol{b} y^{m-1} \frac{\partial y}{\partial x} = r - i \tag{6-7}$$

where $\boldsymbol{b} = \boldsymbol{a}^{1/2}/n$, and $m = 2$ for the last term in Eq. (6-6). Equation (6-7) is solved explicitly as follows (for uniform $\boldsymbol{b}$)

$$y^{t+\Delta t} = y^t - \left\{ \boldsymbol{b} y^t \frac{y^t_{right} - y^t_{left}}{x_{right} - x_{left}} - (r - i) \right\} \Delta t \tag{6-8}$$

where subscripts *left* and *right* refer to the respective neighbor nodes of the node under consideration, and x is the horizontal position of the node.

Thus far, we have not considered the maximum possible infiltration rate. The maximum infiltration rate I_m follows simply from Darcy's law. Consider the CV method used in FUSSIM2. The node nearest to the soil surface is denoted by subscript 1, and the node below it is denoted by subscript 2. The pressure head h_1 at z_1 is the current value of the pressure head when there is no ponding, or is equal to the ponding height y when there is ponding. I_m follows from

$$I_m = -K \frac{h_2 - h_1}{z_2 - z_1} + K \tag{6-9}$$

For K we take the geometric average of $K(h_1)$ and K_s.

It now comes to decide what the true boundary condition will be at the soil surface. If the rainfall rate minus the actual evaporation rate (denoted as r) is larger than I_m, then $i = I_m$. However, according to van Dam *et al.* (1997) r equals I_m only when the following two restrictions are met: $r > I_m$ AND $r > K_s$, where K_s is the hydraulic conductivity at saturation of the soil at the surface. If not both restrictions are met, $i = r$. This extended criterion is used here as well

$$
\begin{aligned}
&\text{if} \quad r > I_m \quad \text{and} \quad r > K_s \quad \text{then} \\
&\qquad i = I_m \\
&\text{else} \\
&\qquad i = r
\end{aligned}
\tag{6-10}
$$

Now all parameters appearing in Eq. (6-8) are known.

For the case $\boldsymbol{b} = 0$ (no slope) or $y^t = 0$ (no ponding) (or no x-gradient in y) Eq. (6-8) reduces to

$$y^{t+\Delta t} = y^t + (r - i)\Delta t \tag{6-11}$$

Then y increases when $r > i$. In that case, since i is always smaller than or equal to r, Eq. (6-11) does not result in lowering of y. From Eq. (6-8) it may result that y lowers due to overland flow, but not due to net infiltration. We will treat lowering of y due to infiltration as follows.

When ponding occurs, i.e. $y > 0$, the type of boundary condition at the soil surface is no longer flux determined, but it will be pressure head determined. Thus a change of boundary type condition must occur (from Dirichlet to Neumann). The prescribed pressure head will be equal to the height of the ponded water layer, i.e. $h_\Gamma = y$. After solving the flow problem inside the soil, a new h distribution is obtained. Then the resulting flux density across the soil surface q_{z0}, providing the prescribed pressure head condition, can be computed. However, q_{z0} is *a-priori* unknown. We applied the following strategy. When in Eq. (6-10) the second rule holds, we added a new restriction: if $Y > 0$ AND $r < I_m$, then $i = I_m$. It appeared in a test case, that for not too small values of Y indeed $i = q_{z0}$. Thus Eq. (6-10) is now written as

if $r > I_m$ and $r > K_s$ then

$\qquad i = I_m$

else

$\qquad$ if $y > 0$ and $r < I_m$ then $\qquad\qquad\qquad\qquad\qquad$ (6-12)

$\qquad\qquad i = I_m$

$\qquad$ else

$\qquad\qquad i = r$

Now it is possible that $r < i$ (middle condition in Eq. (6-12)), so that according to Eq. (6-11) y reduces.

To prevent to large ponding heights under non-sloping conditions (but also under sloping conditions) a maximum ponding height y_m is introduced. Whenever y becomes larger than y_m, y is set to y_m, and the remaining amount of water is considered as (immediate) runoff. During computations, however, y can be larger than y_m.

Of course, y can not become negative, it can only become zero at the time when ponding disappears.

6.3   Implementation in FUSSIM2

Prior to the start of the iterations in FUSSIM2 to obtain new estimates for h at time $(t+\Delta t)$ the y distribution is computed using the old values for h, i.e. h^t. When $h^{t+\Delta t}$ is obtained, the y distribution is computed now using the newest h values. If y has changed, the top boundary condition is changed and new values for h are computed. This iterative process continues until y is constant. Convergence in y is reached whenever the condition

$$\frac{y_l - y}{y + 100} < e_y \qquad\qquad\qquad\qquad\qquad (6-13)$$

is reached (in analogy with convergence criteria used elsewhere in FUSSIM2, Heinen and de Willigen, 1998), where y_l is the previous value of y and e_y is some small number, i.c. $e_y = 10^{-4}$.

6.4   Examples

6.4.1   Case 1

Ponding in a one-dimensional case (surface area 30 cm^2) was simulated for 4 days, with rainfall rates of 1, 2, 20, and 0 cm/d, respectively. No evapotranspiration was

considered. The profile depth was 100 cm, with h initially in equilibrium with $h = 0$ cm at the bottom. At the bottom h was kept at zero (constant ground water level at $z = 100$ cm). In Figure 6-1 the cumulative amounts of rain, actual infiltration (Qtop) and runoff are given. Ponding started at $t = 1.007$ d (lines of rain and Qtop start to deviate) and ended at $t = 3.884$ d (line for Qtop becomes horizontal). Runoff occurred during the third day, when excessive rainfall occurred. The time course of change of y is shown in Figure 6-2. In this case the maximum ponding height was $y_m = 1$ cm.
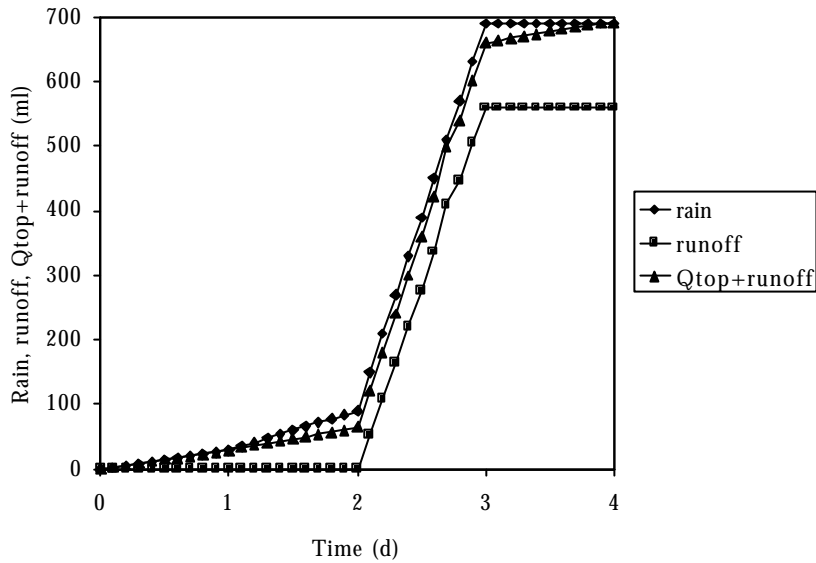
Figure 6-1. Cumulative rain, simulated cumulative runoff and simulated cumulative sum of net entry into the soil (Qtop) and runoff for a one-dimensional situation.
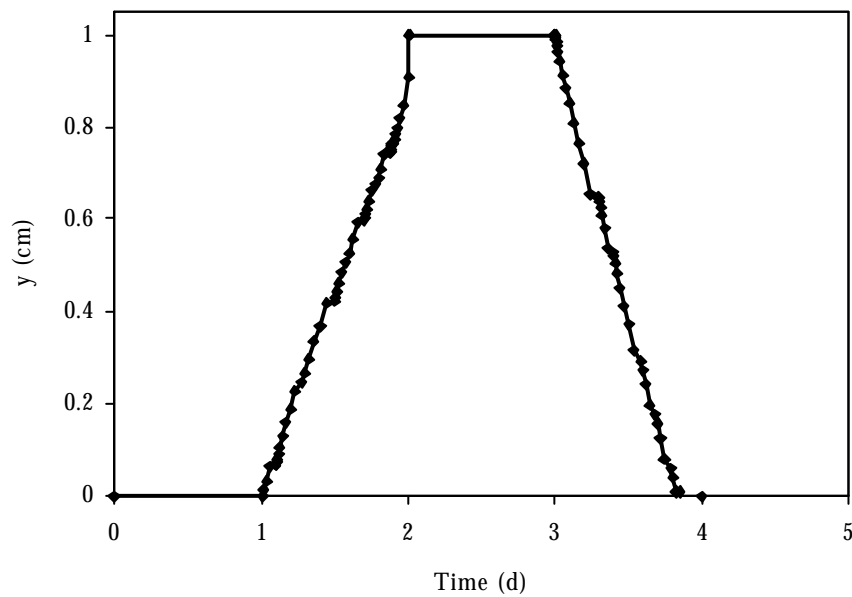
Figure 6-2. Simulated ponding height y as a function of time for the one-dimensional situation.

6.4.2 Case 2

In a second case a sloping surface is considered (two-dimensional case). A soil profile of width 100 cm is at $x = 0$ cm 67.5 cm thick, and at the right ($80 < x < 100$ cm) it is 100 cm thick. The slope **a** from $x = 0$ cm to $x = 80$ cm is 0.5 cm/cm, and the surface roughness $n = 0.03$. Simulation was carried out for 4 days with the same rainfall rates and initial and bottom conditions as used in case 1. In Figure 6-3 the cumulative amounts of rain, actual infiltration (Qtop) and runoff are given. Ponding started at $t = 1.0$ d (lines of rain and Qtop start to deviate) and ended at $t = 4.0$ d (line for Qtop becomes horizontal). Runoff occurred during the third day, when excessive rainfall occurred. The time course of change of y for several positions x is shown in Figure 6-4. In this case the maximum ponding height was $y_m = 1$ cm. There are only small differences in y at the different positions x.
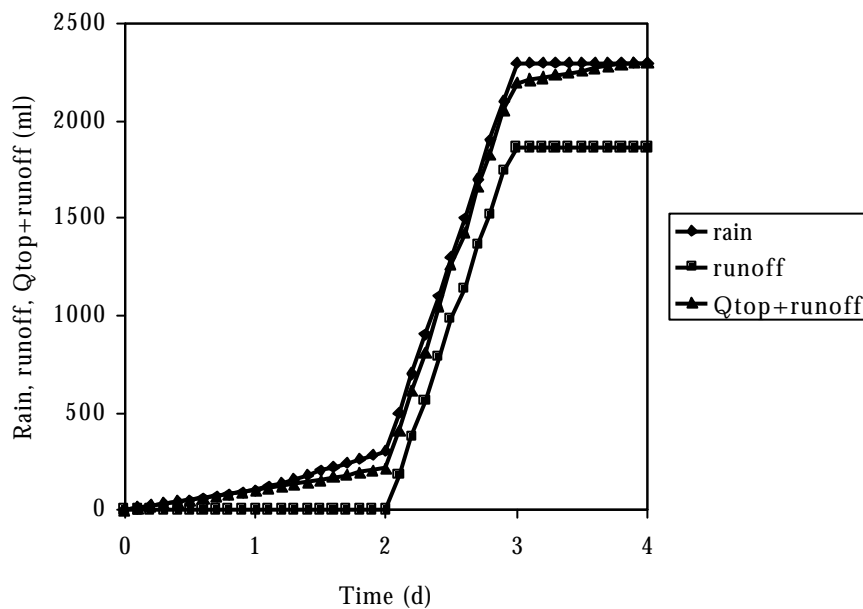
Figure 6-3. Cumulative rain, simulated cumulative runoff and simulated cumulative sum of net entry into the soil (Qtop) and runoff for a two-dimensional sloping situation.
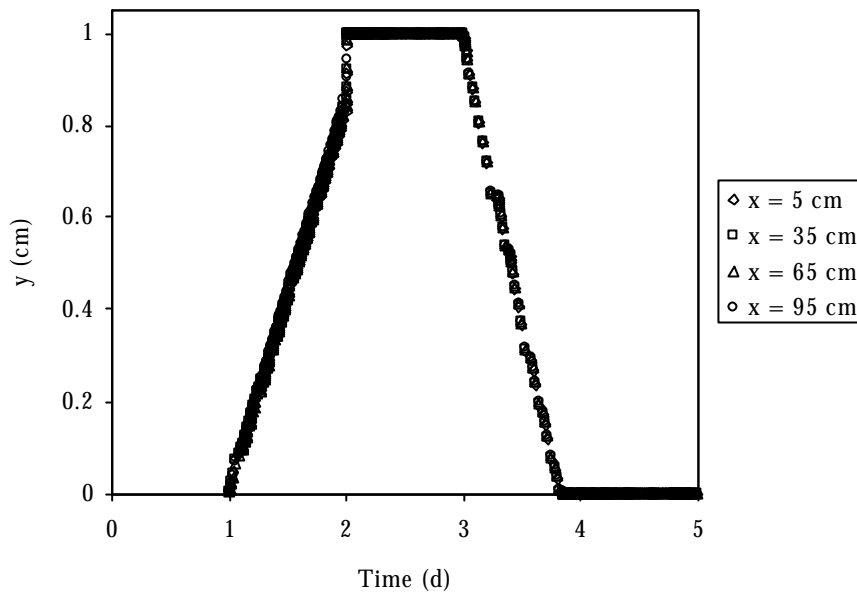
Figure 6-4. Simulated ponding height y as a function of time at four horizontal positions x *for the two-dimensional sloping situation.*

6.5 References

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7 Drain according to the Vimoke concept in FUSSIM2

Marius Heinen, Falentijn Assinck, Bram de Vos

7.1 Introduction

Boundary condition have a large impact on water flow in soils. Drain tubes represent a special boundary. In literature several approaches are described to incorporate a drain in simulation models for water flow (e.g. Fipps *et al*, 1986). In this document we describe how a drain is incorporated in the simulation model FUSSIM2 (Heinen and de Willigen, 1998). We have chosen for the Vimoke concept (Vimoke and Taylor, 1962; Vimoke *et al*., 1963), which is used in other simulation models as well (e.g. Simunek *et al*., 1994; Nieber and Feddes, 1999).

This chapter describes how the Vimoke concept is incorporated in the FUSSIM2 simulation model of Heinen and de Willigen (1998). This chapter is not meant to discuss and describe alternatives for representing drains as a boundary (see e.g. Fipps *et al*, 1986). It also does not discuss all features of the Vimoke concept. This chapter also does not describe the actual concepts of the radial flow towards the drain, and the implications how this should be incorporated in the drain boundary condition.

7.2 Theory

Several decades ago, when computer simulation models were not yet used for studies of water movement in soils, electrical analog experiments were carried out instead. Vimoke and Taylor (1962) and Vimoke *et al*. (1963) reasoned that drains could be represented by nodal points in a regular finite element mesh (in FUSSIM2 the control volume CV), provided that adjustments are made for the hydraulic conductivity K (LT^{-1}) of the neighboring elements. The adjustments should correspond to changes in the electrical resistance of the conducting paper, surrounding the drain node, according to

$$K_{drain} = K C_d \qquad (7\text{-}1)$$

where

K_{drain}	the adapted hydraulic conductivity	LT^{-1}
C_d	the Vimoke correction factor	-

The Vimoke correction factor C_d depends on the ratio of the effective radius r (L) of the drain and the side length D (L) of the CV surrounding the drain node, according to

$$C_d = \frac{Z_0^{'}}{Z_0} = \frac{\sqrt{m_0/e_0}}{138\log_{10} r_d + 6.48 - 2.34a - 0.48b - 0.12c} \tag{7-2}$$

where

$Z_0^{'}$	the characteristic impedance of vacuum	≈ 376.7 Ohm
m_0	the permeability of vacuum	$1.2566 \; 10^{-6}$ H m^{-1}
e_0	the permittivity of vacuum	$8.8542 \; 10^{-12}$ F m^{-1}
Z_0	the characteristic impedance of a transmission line analog of the drain	Ohm

The coefficients in Eq. (7-2) are given by

$$r_d = \frac{D}{r} \tag{7-3}$$

$$a = \frac{1 + 0.405 r_d^{-4}}{1 - 0.405 r_d^{-4}} \tag{7-4}$$

$$b = \frac{1 + 0.163 r_d^{-8}}{1 - 0.163 r_d^{-8}} \tag{7-5}$$

$$c = \frac{1 + 0.067 r_d^{-12}}{1 - 0.067 r_d^{-12}} \tag{7-6}$$

Real drain tubes have a limited amount of openings through which water can enter the drain. Therefore, r will be smaller than the actual drain radius. We assume that a drain is present in a single square CV with side length D, i.e. $r < D$ and $r_d > 1$. Figure 7-1 shows the relationships between C_d, a, b, and c versus r_d for $r_d \in$ [1,10]. It is obvious that C_d for a large range of r_d is larger than 1, which means that $K_{drain} > K$. C_d becomes less than 1 for $r_d \geq 506.1$.
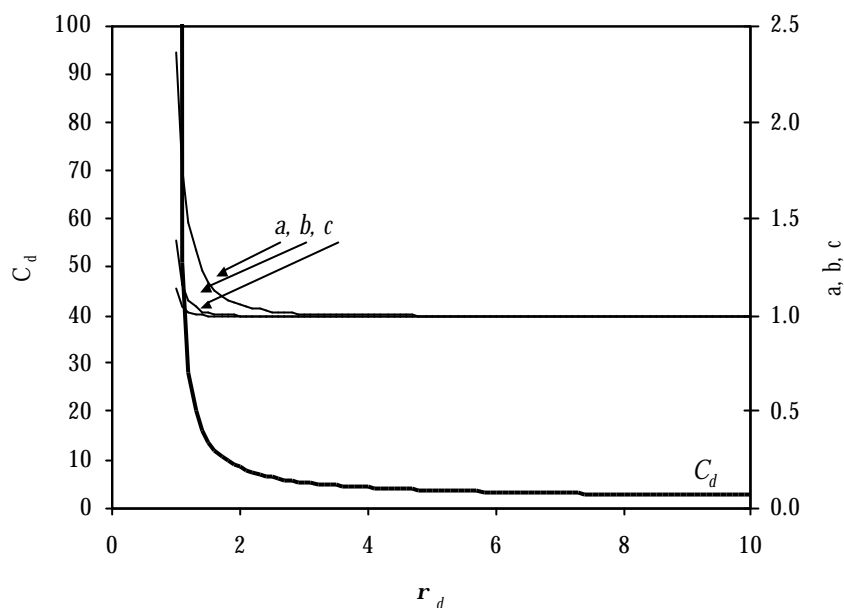
Figure 7-1. C_d, a, b and c as a function of $\mathbf{r}_d$ according to Eqs. (7-2)-(7-6).

In the drainage literature the effective drain radius concept is discussed. There are ways to calculate r from the number and size of the small openings in the drain tube (Mohammad and Skaggs, 1983). It is to the user of FUSSIM2 to decide how to interpret r. It can be seen as a calibration parameter or computed according to theories. Its value may be as small as a few millimeters (J. A. de Vos, pers. comm.). Others determine the effective drain radius from the entrance resistance of drains (see e.g. Dierckx, 1999).

Simunek *et al.* (1994) reported from the literature and their own experience that an additional correction on C_d is required, according to

$$C_d = \frac{C_d}{CF} \tag{7-7}$$

They suggest *CF* to be 2 to 4. Comparing numerical results to an analytical solution of Kirkham (1949), Simunek *et al.* (1994) concluded that *CF* = 4. In that case C_d becomes less than 1 for $r_d \geq 4.5379$. Below in section 7.5 our own experience with the factor *CF* is discussed.

It should be noted that single CV representation of the Vimoke concept has not been studied extensively. We like to quote Simunek *et al.* (1994; p. 30): "*… further studies of the single grid point representation of a subsurface drain may be needed, especially for transient variably-saturated flow conditions.*"

The boundary condition itself is treated comparable to a seepage face. If the drain is empty (i.e. drain outlet above ditch water level), water can only flow into the drain when the soil surrounding the drain is saturated, otherwise the drain is a no-flow

boundary. In the latter case the soil surrounding the drain just acts as normal soil (with adjusted K). In case the drain is full (drain outlet below ditch water level), flow into drain can only occur when the pressure head of the CV representing the drain is larger than the ditch water level, otherwise subsurface infiltration will occur.

If at the beginning of a new time step there is net flow into the CV representing the drain, and the drain outlet is above ditch water level, the condition $h = 0$ is set for this CV, and the drain is running. In case the drain outlet is below the ditch water level, the condition $h = h_{drain}$ is set for this CV, with h_{drain} being the ditch water level above the drain outlet. At the end of the time step, the flow into (or out of) the drain is computed as the net inflow into the CV representing the drain with h of that CV as set as described above.

7.3 Implementation in FUSSIM2

A separate subroutine is written which deals with the representation of a drain as a Vimoke boundary condition. It consists of the following important sections.

7.3.1 Initialize

Read number of Vimoke drains (if zero, all other sections in this subroutine will not be effective; currently maximum 1 drain can be used), read the coordinates of each drain (column and row numbers), read C_d correction factor (-), read effective drain radius r (cm), and read time table of ditch water levels above drain outlet or drain depth.

Check if the CV representing the drain is a square (if CV is not at the boundary), or half a square (if CV is at the boundary but not at the corner), or a quarter of a square (if CV is at the corner). Compute Z_0', a, b, c and $\mathbf{r}_d$. Since the boundary condition is implemented in FUSSIM2 through the existing IINTRN, ITOP, IBOTTOM, ILEFT, IRIGHT variables, the initial values of IINTRN, ITOP, IBOTTOM, ILEFT, IRIGHT are stored, so that these can be used in case the drain is not flowing. For the time being, when the Vimoke drain is on the boundary of the flow domain, it is required that the boundary condition of this CV must be a no-flow boundary.

7.3.2 Compute

Compute K_{drain} (Eqs. (7-1)-(7-2)), compute current net flow into CV, and determine what value h must have. Finally, set IINTRN, ITOP, IBOTTOM, ILEFT, IRIGHT.

In case the Vimoke drain is located at the boundary, the net flux into (or out of) the drain is used as the flow across that boundary (see subroutine FLUXES). As the flux

densities are computed well, the current mass balance computations remain the same.

7.4 Verification against steady-state saturated Kirkham solution

Kirkham (1949) gave an analytical solution for water flow during ponding into equally spaced drain tubes in soil overlying an impervious layer (Figure 7-2). The pressure head h (cm) at any position (x,z) can be computed from (note that Kirkham gave expressions for the total head H)

$$h(x,z) = t + d + qG(x,z) - z \tag{7-8}$$

where q is a flux coefficient (cm) given by

$$q = -\frac{(t+d-r)}{F} \tag{7-9}$$

and the functions $G(x,z)$ and F are given by

$$G(x,z) = \sum_{m=-\infty}^{\infty} \ln \left[\left(\frac{\cosh\left(\dfrac{p(x-ma)}{2h}\right) - \cos\left(\dfrac{pz}{2h}\right)}{\cosh\left(\dfrac{p(x-ma)}{2h}\right) + \cos\left(\dfrac{pz}{2h}\right)} \right) \left(\frac{\cosh\left(\dfrac{p(x-ma)}{2h}\right) + \cos\left(\dfrac{p(z-2d)}{2h}\right)}{\cosh\left(\dfrac{p(x-ma)}{2h}\right) - \cos\left(\dfrac{p(z-2d)}{2h}\right)} \right) \right] \tag{7-10}$$

and

$$
\begin{aligned}
F &= \sum_{m=-\infty}^{\infty} \ln \left[\left(\frac{\cosh\left(\dfrac{pma}{2h}\right) - \cos\left(\dfrac{pr}{2h}\right)}{\cosh\left(\dfrac{pma}{2h}\right) + \cos\left(\dfrac{pr}{2h}\right)} \right) \left(\frac{\cosh\left(\dfrac{pma}{2h}\right) + \cos\left(\dfrac{p(2d-r)}{2h}\right)}{\cosh\left(\dfrac{pma}{2h}\right) - \cos\left(\dfrac{p(2d-r)}{2h}\right)} \right) \right] \\
&= -2 \ln \left(\frac{\tan\left(\dfrac{p(2d-r)}{4h}\right)}{\tan\left(\dfrac{pr}{4h}\right)} \right) + \\
&\quad -2 \sum_{m=1}^{\infty} \ln \left[\left(\frac{\cosh\left(\dfrac{pma}{2h}\right) + \cos\left(\dfrac{pr}{2h}\right)}{\cosh\left(\dfrac{pma}{2h}\right) - \cos\left(\dfrac{pr}{2h}\right)} \right) \left(\frac{\cosh\left(\dfrac{pma}{2h}\right) - \cos\left(\dfrac{p(2d-r)}{2h}\right)}{\cosh\left(\dfrac{pma}{2h}\right) + \cos\left(\dfrac{p(2d-r)}{2h}\right)} \right) \right]
\end{aligned} \tag{7-11}
$$

respectively. The parameters a, d, h, r, t, x and z (all in cm) appearing in Eqs. (7-8)-(7-11) are explained in Figure 7-2. The origin of the (x,z) coordinate system is located at the center of the drain, with x positive to the right, and z positive upwards (Figure 7-2). The drainage outflow rate Q (cm³ water per cm length of the drain per day) is obtained from

$$Q = 4pqK_s \qquad (7\text{-}12)$$

where
   K_s the hydraulic conductivity at saturation   cm d⁻¹
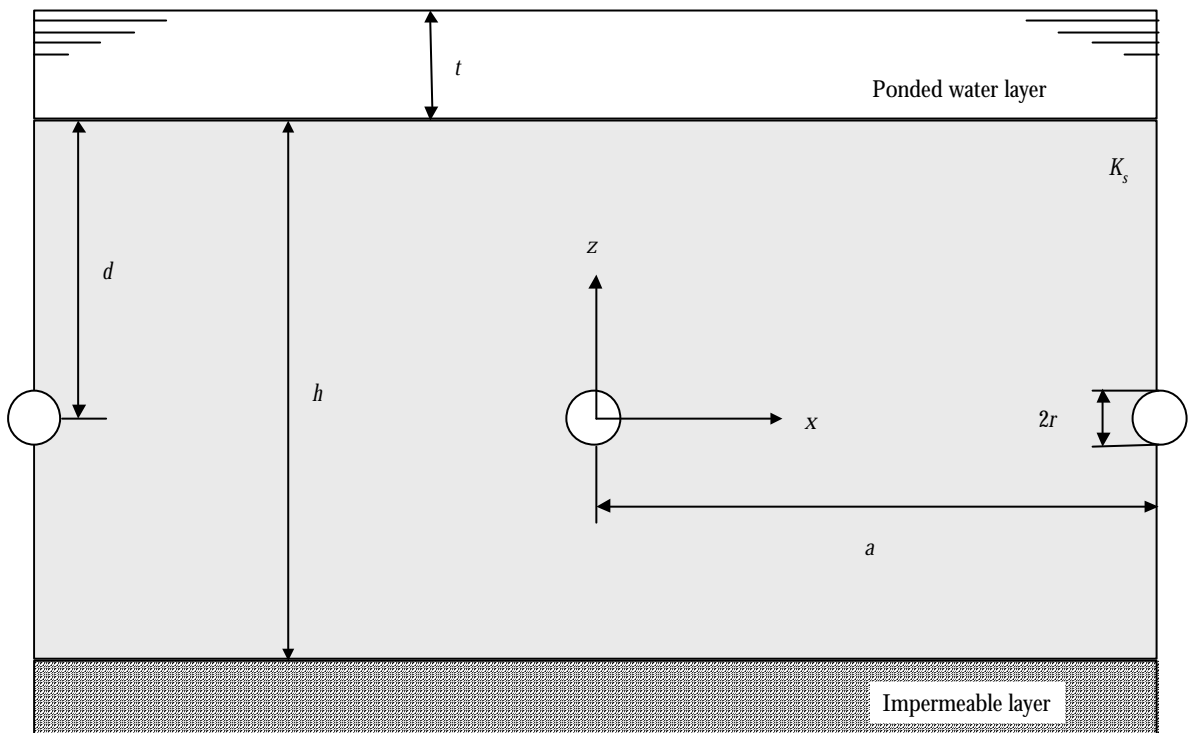
Figure 7-2. Cross sectional view of a soil with equally spaced drains with water ponding at the surface and an impermeable layer at the bottom (after Kirkham, 1949).

This equation holds for a homogeneous soil profile only. For small drain spacing Kirkham (1949) gave alternative expressions for Eqs. (7-8)-(7-11) (see Appendix at the end of this chapter). In the example below, the two solutions gave identical results.

7.4.1 Simulation

We consider a soil profile of 51 cm deep (= h) and 42 cm wide (= a), with a drain located at depth 36 cm (= d) and midway between the left and right boundaries. The radius of the drain was 1 cm (= r). The left, right and bottom boundaries are all no-flow boundaries. At the soil surface a fixed pressure head was set equal to $h = 0$ cm (just ponding; $t = 0$ cm). Initially the soil profile is at equilibrium with $h = +51$ cm at the bottom. The dimensions of the Control Volumes were 2x2 cm^2 (i.e. $D = 2$ cm), except for the first layer which had a thickness in z of 1 cm. The hydraulic conductivity at saturation was $K_s = 14.07$ cm d^{-1}. The soil profile remained saturated, and steady-state was almost directly simulated. At first, two simulations were carried out, i.e. the first with $CF = 1$ and the second with $CF = 4$. Later, a detailed analysis was carried out to find out which CF should be used.

7.4.2 Results

Figure 7-3 presents the simulated h distributions for CF equal to 1 or 4 (upper two graphs) as well as the analytical solution of Kirkham (1949) in the lower left graph (Eq. (7-8)). The simulated distributions are close to the analytical solutions, but not exactly the same. In the next section (section 7.5) the choice of the factor CF is elaborated on in detail. Running ahead of the result presented there, the best agreement between simulated and analytical solutions was obtained for $CF = 2.07$ (lower right graph in Figure 7-3). The average of the relative differences between simulated and analytical h-distributions were for $CF = 1$, 2.07 and 4 equal to 9.19 10^{-2}, 8.20 10^{-4} and -7.61 10^{-2}, respectively.

Depth (cm)
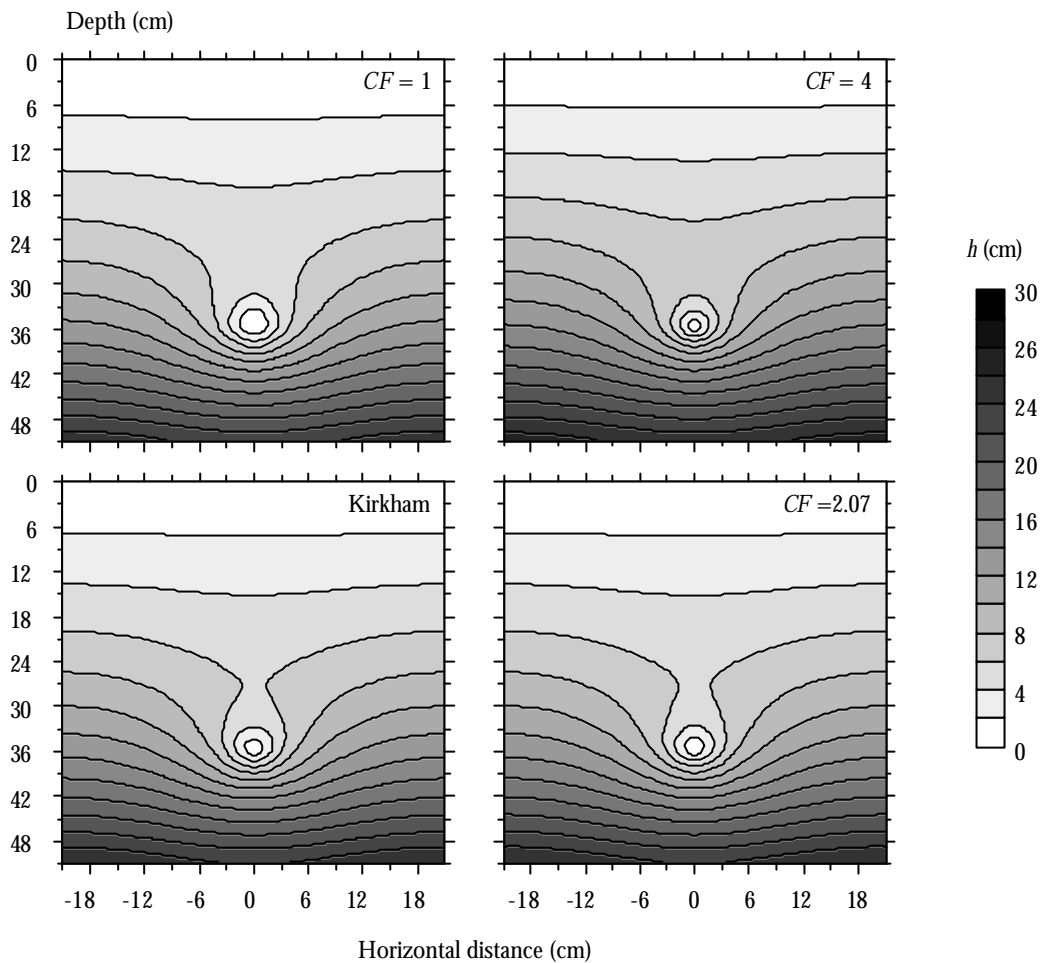
Figure 7-3. Analytical (lower left graph) and three simulated pressure head distributions for water flow with water ponding at the soil surface with a tile drain represented as a Vimoke drain using FUSSIM2. In each of the three simulations a different correction factor CF was used: 1 (upper left graph), 4 (upper right graph), and 2.07 (lower right graph). Other parameters were: a = 42 cm, d = 36 cm, h = 51 cm, t = 0 cm, r = 1 cm, D = 2 cm, and K_s = 14.07 cm d^{-1}.

7.5   On CF

Above in section 7.2 a correction factor for C_d was introduced: *CF* (Eq. (7-7)). As was stated there, there is not yet insight in why a correction factor is needed, and, if so, what its exact value must be. Since in the first attempt in comparing simulated with analytical pressure head distributions (section 7.4), the proposed value of 4 (Simunek *et al.*, 1994; their Figure 4.1) does not apply to the situation considered in this chapter. Therefore, we decided to carry out an analysis to determine if *CF* is related to *r* or better $\boldsymbol{r}_d$. For the example described above we carried out simulations for *CF* = 1, 2, 3, …, 20 and for *r* = 1, 0.5, 0.2, 0.1, 0.05, 0.02, 0.01, 0.005, 0.002, and 0.001 cm (*D* = 2 cm). The analytical *h* distributions as well as the analytical *Q* values were computed. For both *h* and *Q* the (sum of) squared differences were considered

$$ssq_h = \sum \left(\frac{h_{sim} - h_{an}}{h_{an}} \right)^2 \tag{7-13}$$

and

$$ssq_Q = \sum \left(\frac{Q_{sim} - Q_{an}}{Q_{an}} \right)^2 \tag{7-14}$$

where the summation in Eq. (7-13) refers to all nodes in the simulated soil domain. Both ssq_h and ssq_Q showed nice minima in the r_d-CF space. As an example, the contour distribution of ssq_Q is given in Figure 7-4; that of ssq_h looked similar. Since both ssq_Q and ssq_h gave the same minima in the r_d-CF space, the following analysis is carried out on Q only.
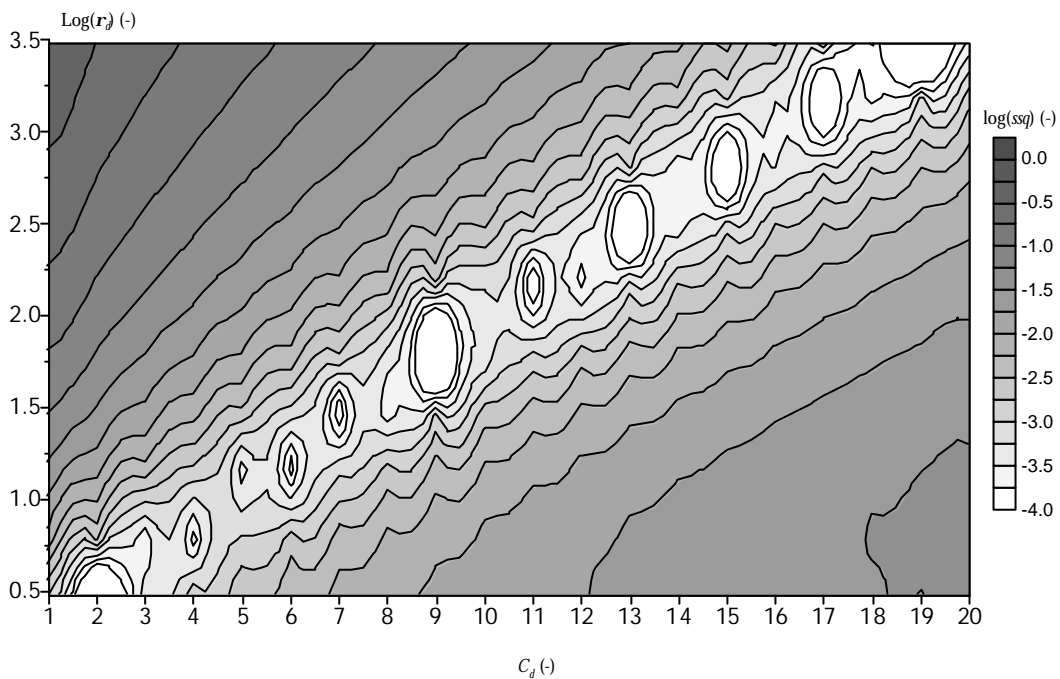
Figure 7-4. Contour plot of log(ssq_Q) for different combinations of C_d and r_d.

Using linear interpolation, that value of CF was obtained for which simulated Q equaled the analytical value. Next, through regression analysis a relationship between CF and $\log(r_d)$ was obtained. Both a linear fit and a fourth order polynomial were determined as described by (Figure 7-5)

$$CF = a + b\log(r_d)\left\{ + g\log(r_d)^2 + d\log(r_d)^3 + e\log(r_d)^4 \right\} \tag{7-15}$$

The fitted values of the parameters for both the fourth order polynomial and for the linear fit are presented in Table 7-1 (case 1). Both fits and the computed CF values are given in Figure 7-5. Remember that the points in Figure 7-5 were estimated and are thus not exact.

For the example given above $r_d = 2$, so that according to Eq. (7-15) (fourth order polynomial) $CF = 2.07$, which was the case shown in Figure 7-3. The linear fit deviated most at $r_d = 1$, where it yields $CF = 1.80$. In general, the relative difference in Figure 7-5 for the fourth order polynomial is less than 0.1%, while for the linear fit this is less than 2% ($r_d > 4$), except for small values of r_d, e.g. at $r_d = 1$ it is 13%.
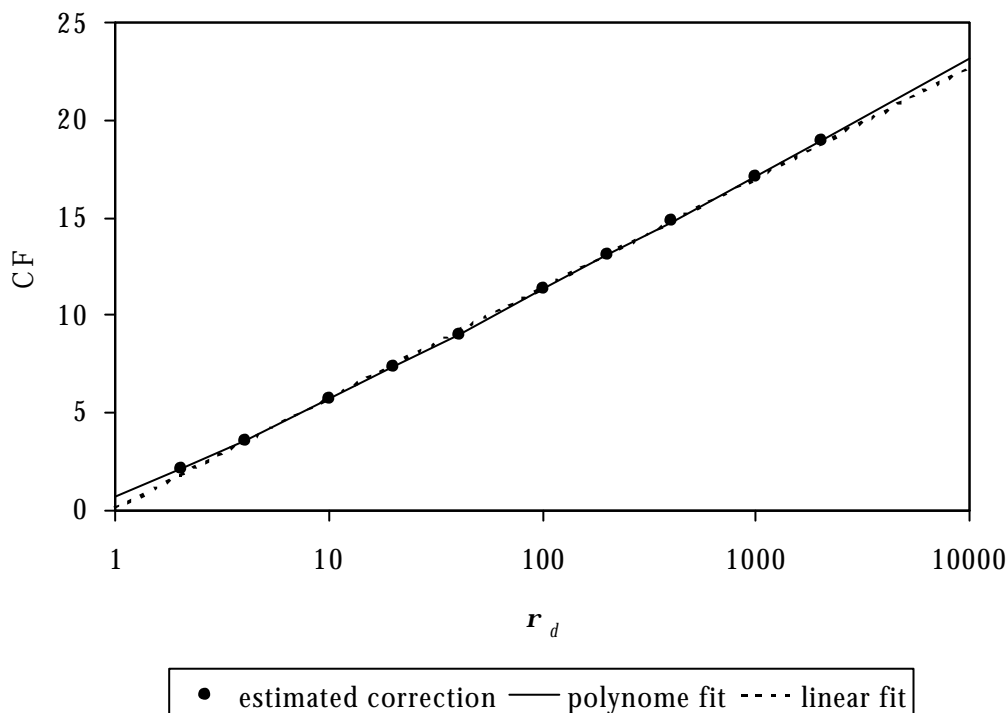
Figure 7-5. Fitted relationship between CF and r_d.

Table 7-1. Parameters for the fourth order polynomial or linear regression Eq. (7-15) for the two cases as described in the text.

Parameter	Case 1		Case 2	
	4th order polynomial	Linear	4th order polynomial	Linear
a	0.738558	0.098256	0.123857	-0.111594
b	4.136663	5.664468	5.304643	5.758459
g	1.028875		0.196783	
d	-0.281507		-0.018366	
e	0.029084		-0.001307	

In order to see if such a relationship is dependent on the problem studied, we have carried out the same analysis for the situation of $a = 66$ cm, $d = 49$ cm, $h = 80$ cm, and $t = 10$ cm. For this case the fitted parameters of Eq. (7-15) are given in Table 7-1 (case 2). The values of the parameters differ between the two cases, but visually there

are hardly any differences. It appears that the shape of the flow domain has no effect on the relationship between CF and r_d. Equation (7-15) may serve as to obtain an estimate for CF. However, care must be taken, since the results are only obtained for two situations. Furthermore, it should be noted that single Control Volume representation of the Vimoke concept has not been studied extensively, especially not for variably saturated situations. We like to quote Simunek *et al.* (1994; p. 30): "*… further studies of the single grid point representation of a subsurface drain may be needed, especially for transient variably-saturated flow conditions.*". In section 7.7 we present a transient, variably saturated problem.

Finally, one simulation was carried out for the case $a = 1200$ cm, $d = 95$ cm, $h = 197.5$ cm, $r = 1$ cm, $t = 0$ cm, $D = 5$ cm and $K_s = 14.07$ cm d^{-1}. From Eq. (7-15) with $r_d = 5$, CF was computed as $CF = 4.043$. The analytical outflow from the drain (Eq. (7-12)) was $Q = 1522.0$ cm^3 cm^{-1} d^{-1} and the simulated outflow was 1512.3 cm^3 cm^{-1} d^{-1}, thus the relative difference equals only –0.6%. The h distributions were also nearly equal with the average relative difference being 7.68 10^{-4}, which is similar to the average difference observed in the section 7.4. Thus, also for a large saturated flow domain Eq. (7-15) seems to yield a good estimate for CF. In general, the differences are largest around the drain, especially above and below the drain. For a given horizontal position z there is a trend in the differences, with the differences largest at the position of the drain $x = 0$ cm.

7.6 Steady-state variably saturated example

The previous example described a steady-state saturated situation. Before going to a transient variably saturated situation we give here an example of steady-state variably saturated situation. We will present the position of the water table for three values of effective drain radius r (2.5 cm, 0.025 cm, 0.00025 cm) without (i.e. $CF = 1$) and with correction factor CF as computed according to Eq. (7-15). For comparison we show also the ground water level according to the Hooghoudt (1940) formula. For a situation with an impermeable layer at some depth below the drain (c.f. Figure 7-2), the Hooghoudt formula reads (Hooghoudt, 1940; his equation (98) on page 593)

$$s = \frac{8Kd_e m_0 + 4Km_0^2}{L^2} \tag{7-16}$$

where

m_0	maximum ground water level between two drains	cm
L	drain distance (= a in Figure 7-2)	cm
s	steady-state rainfall intensity	cm d^{-1}
K	hydraulic conductivity at saturation	cm d^{-1}
d_e	equivalent thickness of soil layer between drain and impermeable layer	cm

From Eq. (7-16) it follows that m_0 can be computed as

$$m_0 = -d_e + \sqrt{d_e^2 + \frac{sL^2}{4K}} \qquad (7\text{-}17)$$

The equivalent thickness of soil layer between drain and impermeable layer d_e (not to be confused with drain depth d used in Figure 7-2 and section 7.4) can be computed from (Wesseling, 1973; see also van der Ploeg *et al.*, 1999)

$$d_e = \frac{L}{8} \left[\frac{\left(L - H\sqrt{2}\right)^2}{8HL} + \frac{1}{p} \ln\left(\frac{H\sqrt{2}}{2r}\right) \right]^{-1} \qquad (7\text{-}18)$$

where
H actual distance between drain and impermeable layer ($= h - d$ in Figure 7-2)   cm

Hooghoudt's theory implies that the shape of the water table is elliptic. In our case the height of the water table above the impermeable layer $h(x)$ (cm) is given by (e.g. Koopmans, 1995)

$$h(x) = \sqrt{h(0)^2 + \frac{s}{K}\left(Lx - x^2\right)} \qquad (7\text{-}19)$$

where
x	the horizontal distance	cm
$h(x)$	the height of the water table above the impermeable layer	cm
$h(0)$	the height of the water table above the impermeable layer at the drain $= H$	cm

We considered a field with drain spacing $L = 12$ m, profile depth $= 2$ m, drain depth $= 0.975$ m ($H = 1.025$ m, $d_e = 0.7$ m, $m_0 = 0.6$ m), physical drain radius $r = 0.03$ m, a hydraulic conductivity $K = 0.306$ m d^{-1} and a constant rain intensity $s = 0.01$ m d^{-1}. The six ground water levels at steady-state are shown in Figure (7-6). As can be seen from Figure (7-6) there are cases where simulated ground water level and that predicted by Hooghoudt are similar. Of course, Hooghoudt's formula is an estimation of the position of the ground water level and, therefore, cannot be regarded as an analytical solution to which we can verify the Vimoke drain concept. It is generally known that Hooghoudt's formula underestimates the ground water level near the drain. The simulation results always result in a higher ground water level nearby the drain.
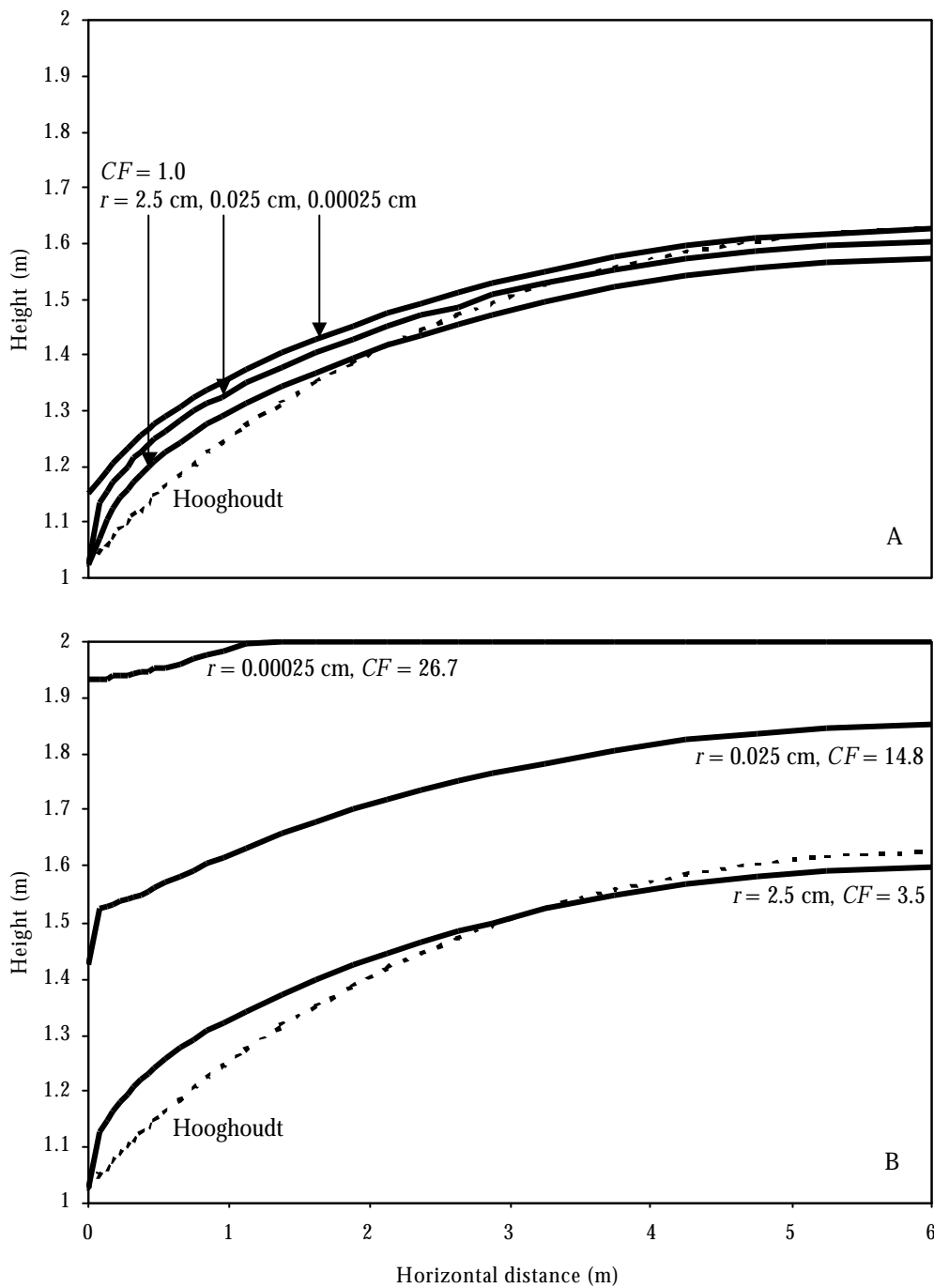
Figure 7-6. Simulated (solid lines) positions of the water table for steady-state variable saturated water flow for three values of r (A) without (CF = 1) and (B) with CF computed according to Eq. (7-15). For comparison the Hooghoudt prediction (Eq. (7-19)) is given as well (broken line).

It can also be seen from Figure (7-6) that the combination $r = 0.025$ cm and $CF = 1$ and the combination $r = 2.5$ cm and $CF = 3.5$ result in nearly the same water table positions. In other words, a certain position of the ground water level can be achieved by either changing r and/or CF. Since both r and CF affect C_d and thus

affect K of the control volume where the drain is located, the question arises whether or not it is necessary to include a correction factor CF in the computations, as the same results can also be achieved by changing r.

7.7   Validation for a transient variably saturated situation

De Vos (1997) measured in detail groundwater level fluctuations and drain discharges (water volume and NO_3 concentration) from a single drain during a leaching season. With a detailed description of a seepage drain he was able to simulate similar patterns as measured. Here we show simulation results for exactly the same situation using the Vimoke drain concept, with and without CF. We used the optimized hydraulic parameters of de Vos (1997; his Table 8.3, using extended van Genuchten-Mualem models as described in Chapter 4 of this report) for the Lovinkhoeve soil profile (de Vos, 1997; his Figure 8.2), and climatic data of de Vos (1997). The effective drain radius r_{eff} (cm) used as the drain radius in the simulation model was calculated from (Dierckx, 1999; his Eqs. (13) and (16) for circular drains)

$$r_{eff} = r \exp\left(-2p a_e\right)$$

$$a_e = \frac{c}{2p^2 r}\left(\ln\left(\frac{c}{pb}\right) - \frac{c}{4pr}\right)$$

(7-20)

where

r	physical drain radius (outer)	cm
c	gap spacing	cm
b	gap width	cm

For $r = 3.75$ cm, $c = 30$ cm and $b = 1$ cm, $r_{eff} = 0.06$ cm. The initial pressure head distribution was that of an equilibrium situation with $h = +84$ cm at the bottom of the soil profile, and the initial NO_3 distribution was taken from de Vos (1997; his Figure 8.12).

Figure 7-7 shows the simulation grid used by FUSSIM. The control volume where the Vimoke drain was located had a typical dimension of $D = 2.5$ cm. Figure (7-8) shows the comparison between simulated and measured water outflow, position of the ground water level midway between two drains and NO_3 concentration of the drain water. The comparison is rather good. The deviation between simulated and measured data is of the same order as de Vos (1997) obtained with his simulation model.
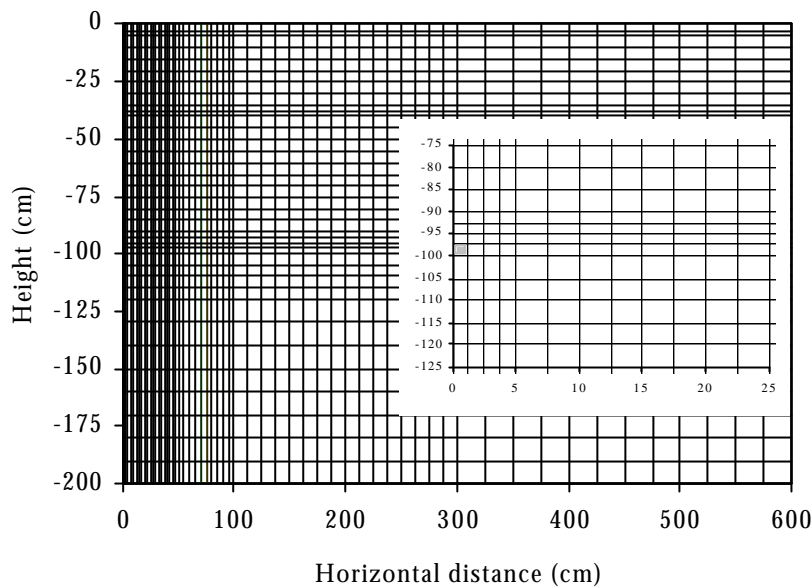
Figure 7-7. Grid lay-out used in the simulation. In-set shows grid around the Vimoke drain (gray rectangle).

In an earlier attempt to carry out this validation we used a coarser grid. This resulted in similar patterns, except that at three times a peak in outflow occurred at times at which the measured data did not show peaks. This must be due to numerical dispersion. Therefore, care must always been taken in choosing a representative grid when using the Vimoke drain concept.

The simulations described above used $CF = 1$. In a run with CF computed according to Eq. (7-14) for given r about exactly the same results were obtained. The main difference was that the run time was much larger (about 4 to 4.5 times). Combining this experience and that of section 7.6 we conclude that in future use of the Vimoke drain concept the resistance of the control volume where the drain is located can best be done by changing only the value of the effective drain radius r and have $CF = 1$, and use a fine enough grid of the soil domain. To check if the grid is dense enough, the sensitivity for this density should be tested. An acceptable grid density is found when preset criteria on accuracy are met.
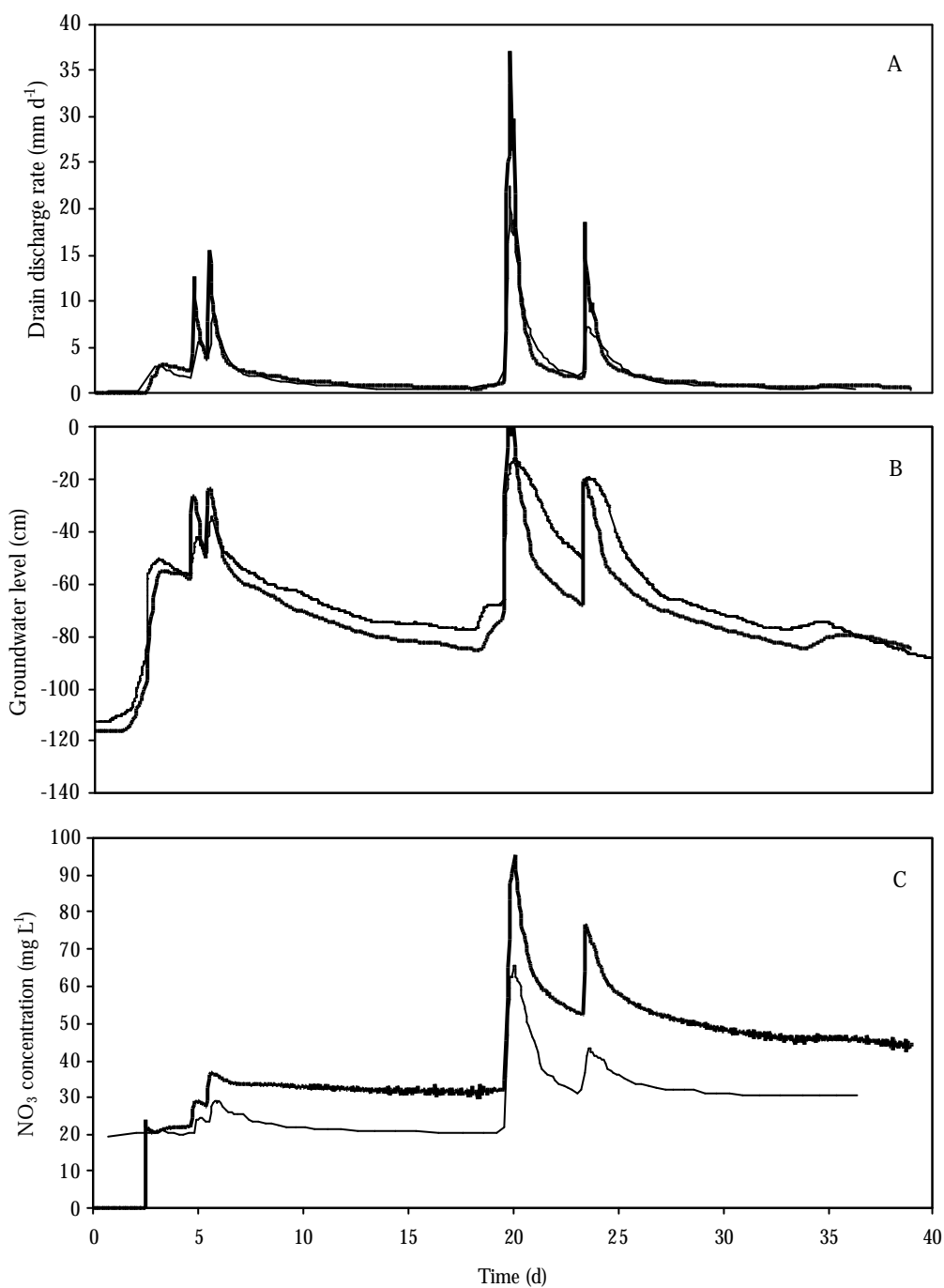
Figure 7-8. Simulated (thick line) and measured (thin line) (A) drain discharge rate, (B) groundwater level midway between two drains, and (C) NO₃ concentration of the drain water as a function of time.

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7.9   Appendix

Kirkham (1949) gave also analytical solutions for the case of close drain spacing. These solutions can be written analogous to Eqs. (7-8)-(7-11). The pressure head follows from

$$h_a(x,z) = t + d + q_a G_a(x,z) - z \tag{7-21}$$

where q_a is given by

$$q_a = -\frac{(t+d-r)}{2 F_a} \tag{7-22}$$

and the functions $G_a(x,z)$ and F_a are given by

$$G_a(x,z) = \sum_{n=-\infty}^{\infty} (-1)^n \ln\left(\frac{\cosh\left(\frac{2p(z-2nh)}{a}\right) - \cos\left(\frac{2px}{a}\right)}{\cosh\left(\frac{2p(z-2d-2nh)}{a}\right) - \cos\left(\frac{2px}{a}\right)} \right) \tag{7-23}$$

and

$$F_a = \ln\left(\frac{\sinh\left(\frac{p(2d-r)}{a}\right)}{\sinh\left(\frac{pr}{a}\right)} \right) - \sum_{n=1}^{\infty} (-1)^n \ln\left(\frac{\sinh^2\left(\frac{2pnh}{a}\right) - \sinh^2\left(\frac{pr}{a}\right)}{\sinh^2\left(\frac{2pnh}{a}\right) - \sinh^2\left(\frac{p(2d-r)}{a}\right)} \right) \tag{7-24}$$

respectively.

Kirkham (1949) also presented analytical solutions for the stream function and for the rate of intake at the soil surface.

8   P-adsorption and P-fixation in FUSSIM2

Peter de Willigen and Marius Heinen

8.1   Introduction

P in soil is present in the following three phases:
1.   in solution
2.   at the adsorption complex
3.   fixated in Fe+Al (hydr)oxides

P in phases 1 and 2 is called the labile fraction of P. Transport of P occurs in the solution phase only. Instantaneous equilibrium exists between P in phase 1 and phase 2. Fixation into phase 3 is slow process and is assumed to be dependent on the difference between amount of P in solution and P already fixated.   In what follows we will describe how P transport and P distribution in soil is computed in the simulation model FUSSIM2.

8.2   The general transport equation

The governing transport equation for P is given by (*cf.* Heinen, 1997)

$$\frac{\partial Q}{\partial t} = -\nabla \cdot q_s - S_s + \frac{\mathrm{d}F}{\mathrm{d}t} \tag{8-1}$$

where
Q	total amount of P	mg cm^{-3}
t	time	d
$\nabla\cdot$	divergence	cm^{-1}
q_s	solute flux density	mg cm^{-2} d^{-1}
S_s	root uptake	mg cm^{-3} d^{-1}
$\mathrm{d}F/\mathrm{d}t$	fertilization rate	mg cm^{-3} d^{-1}

The total amount Q is given by

$$Q = \boldsymbol{q}c + Q_A + Q_F = P_{i,v} + Q_F \tag{8-2}$$

where
c	P concentration in soil solution	mg ml^{-1}
$\boldsymbol{q}$	volumetric water content	ml cm^{-3}
Q_A	amount of P at adsorption complex	mg cm^{-3}
Q_F	amount of P fixated	mg cm^{-3}
$P_{i,V}$	labile amount of P, $P_{i,V} = \boldsymbol{q}c + Q_A$	mg cm^{-3}

In general, cm³ refers to volume of soil, and ml to volume of solution.

8.3 Expression for the new labile amount

Substituting Eq. (8-1) in Eq. (8-2) yields

$$\frac{\partial P_{i,v}}{\partial t} + \frac{\partial Q_F}{\partial t} = -\nabla \cdot q_s - S_s + \frac{\mathrm{d}F}{\mathrm{d}t} \tag{8-3}$$

Rewriting yields

$$\frac{\partial P_{i,v}}{\partial t} = \frac{\partial Q}{\partial t} - \frac{\partial Q_F}{\partial t} \tag{8-4}$$

In Eq. (8-4) we have expressed the time change of labile amount $P_{i,V}$ as a function of time change of P due to transport, uptake and fertilization ($\partial Q/\partial t$) and time change of fixed P ($\partial Q_F/\partial t$). Thus, we assume that all unknowns can be computed based on explicitly known concentration c^t. The new $P_{i,V}$ at time $t+\Delta t$ follows from

$$P_{i,v}^{t+\Delta t} = P_{i,v}^{t} + \left(\left.\frac{\partial Q}{\partial t}\right|_{c^t} - \left.\frac{\partial Q_F}{\partial t}\right|_{c^t} \right)\Delta t \tag{8-5}$$

The new concentration $c^{t+\Delta t}$ is obtained by solving

$$\boldsymbol{q}^{t+\Delta t} c^{t+\Delta t} + f\left(c^{t+\Delta t}\right) - P_{i,v}^{t+\Delta t} = 0 \tag{8-6}$$

where
   f(c)   adsorption isotherm   mg cm⁻³

The concentration $c^{t+\Delta t}$ is found using the ZBRENT method of Press *et al.* (1992). The value of $c^{t+\Delta t}$ is bounded by the range

$$0 \le c^{t+\Delta t} \le \frac{P_{i,v}^{t+\Delta t}}{\boldsymbol{q}^{t+\Delta t}} \tag{8-7}$$

The amount adsorbed then follows from the adsorption isotherm (see below).

8.4 P fixation

For the fixation process we use the three-pool Freundlich-type model of Schoumans (1995; his equation (68)), given by

$$\frac{\partial Q_F}{\partial t} = \sum_{i=1}^{3} a_i \left(K_{F,i} c^{N_i} - Q_{s,i} \right) \tag{8-8}$$

where

Q_F	amount of P fixated, $Q_F = Q_{s,1} + Q_{s,2} + Q_{s,3}$	mg cm^{-3}
$Q_{s,1}$	amount of P fixated in pool 1	mg cm^{-3}
$Q_{s,2}$	amount of P fixated in pool 2	mg cm^{-3}
$Q_{s,3}$	amount of P fixated in pool 3	mg cm^{-3}
a	extinction coefficient	d^{-1}
N	exponent coefficient	-
K_F	fixation coefficient	mg cm^{-3} (mg ml^{-1})$^{-N}$

At given c and known quantities Q_s, the rate MQ_F/Mt can be computed. The new quantities Q_s follow from the individual time rate of changes through integration.

The coefficients K_F are not read directly from an input file but are computed from other supplied parameters according to

$$K_F = b \left(10^3 \right)^N [\text{Al} + \text{Fe}] 31 \cdot 10^{-3} \, r_d \tag{8-9}$$

where

K_F	fixation coefficient	mg cm^{-3} (mg ml^{-1})$^{-N}$
b	fixation parameter	(mg l^{-1})$^{-N}$
$(10^3)^N$	conversion factor to transform b from (mg l^{-1})$^{-N}$ to (mg ml^{-1})$^{-N}$	(mg ml^{-1})$^{-N}$ ((mg l^{-1})$^{-N}$)$^{-1}$
N	exponent coefficient	-
[Al+Fe]	oxalate extractable Al and Fe	mmol kg^{-1}
31	molecular weight of P	mg mmol^{-1}
10^{-3}	conversion factor from kg to g	kg g^{-1}

8.5   P adsorption isotherms

We have implemented two types of adsorption isotherms, i.e. a Langmuir and a Freundlich isotherm. The Langmuir isotherm is given by

$$Q_A = \frac{a_1 b_1 c}{1 + b_1 c} + \frac{a_2 b_2 c}{1 + b_2 c} \tag{8-10}$$

where

a	Langmuir a coefficient	mg cm^{-3}
b	Langmuir b coefficient	ml mg^{-1}

For $c \to \infty$, $Q_A = a_1 + a_2$, so that $a_1 + a_2$ represents the adsorption maximum. Equation (8-10) is a so-called double-Langmuir adsorption isotherm. By setting $a_2 = b_2 = 0$ one obtains the single-Langmuir adsorption isotherm.

The Freundlich isotherm is given by

$$Q_A = Mc^N \tag{8-11}$$

where
N	Freundlich N coefficient	
M	Freundlich M coefficient	mg cm^{-3} (mg ml^{-1})$^{-N}$

For completeness, a linear adsorption isotherm is available, and is given by $Q_A = a_k c$, which can be seen as a special case of the Freundlich isotherm with $M = a_k$ and $N = 1$.

8.6   Computation of P_w

In The Netherlands the P_w value, based on an extraction of soil P with water, is used as a basis for P fertilizer recommendations for arable crops. Van Noordwijk *et al.* (1990) showed that P_w can be computed from the labile amount $P_{i,V}$. $P_{i,V}$ equals the sum of P in solution and P at the adsorption complex, according to

$$P_{i,v} = qc + Q_A \tag{8-12}$$

It is assumed that during the extraction $P_{i,V}$ does not change, that the desorption isotherm is equal to the adsorption isotherm, and that effects of background electrolyte concentration on the desorption/adsorption process may be neglected. Thus, we have

$$P_{i,v} = qc + Q_A = \frac{V_w}{V_s}c^* + Q_A^* \tag{8-13}$$

where
V_w / V_s	water:soil (v:v) ratio used when P_w is determined in soil samples	ml cm^{-3}
c^*	concentration during the determination of the P_w value	mg ml^{-1}
Q_A^*	amount adsorbed for given c^*	mg cm^{-3}

For given $P_{i,V}$ and adsorption isotherm parameters, the value for c^* can be determined from Eq. (8-13) ($Q_A^* = f(c^*)$, *cf.* Eq. (8-6))

$$\frac{V_w}{V_s}c^* + f(c^*) - P_{i,v} = 0 \tag{8-14}$$

The concentration c^* is found using the ZBRENT method of Press *et al.* (1992). The value of c^* is bounded by the range

$$0 \leq c^* \leq \frac{P_{i,v}}{V_w / V_s} \qquad (8\text{-}15)$$

Finally, the value P_w (in mg P_2O_5 per L soil) is computed from c^* according to

$$P_w = c^* 10^3 \frac{V_w}{V_s} \frac{142}{2 \cdot 31} \qquad (8\text{-}16)$$

where
P_w	water-soluble P	mg P_2O_5 L^{-1} soil
10^3	conversion from cm^{-3} soil to L^{-1} soil	cm^3 L^{-1}
142	molecular weight of P_2O_5	mg P_2O_5 $mmol^{-1}$
31	molecular weight of P	mg P $mmol^{-1}$
2	number of moles P per mol P_2O_5	mmol P $mmol^{-1}$ P_2O_5

8.7   The initial situation

In order to start simulation, the initial P distribution must be known. The initial $P_{w,0}$ distribution is chosen as initial condition. From that the initial concentration, initial amount adsorbed, and initial amount fixated are computed.

The initial concentration c_0 is computed from $P_{w,0}$ according to the reversed pathway as described in the section 8.6. For given $P_{w,0}$ c^* can be computed from Eq. (8-16). The labile amount $P_{i,V}$ follows from c^* according to Eq. (8-13) and a description of the adsorption isotherm. Now we have the distribution in the diluted soil sample. The distribution of $P_{i,V}$ over actual soil solution and adsorption complex follows from Eq. (8-13) (in analogy to Eq. (8-14); $Q_0 = f(c_0)$) according to

$$q_0 c_0 + f(c_0) - P_{i,v} = 0 \qquad (8\text{-}17)$$

Equation (8-17) is solved for c_0, knowing that c_0 is bounded by the range

$$0 \leq c_0 \leq \frac{P_{i,v}}{q_0} \qquad (8\text{-}18)$$

From c_0 the initial amount adsorbed $Q_{A,0}$ follows from the adsorption isotherm (Eq. (8-10) or (8-11)).

The initial amount fixated P, $Q_{F,0}$, is computed from c_0 assuming equilibrium. $Q_{F,0}$ is the sum of the initial amounts $Q_{s,0}$ of the three pools, which are computed from

$$Q_{s,1,0} = K_{F,1} c_0^{N_1}$$
$$Q_{s,2,0} = K_{F,2} c_0^{N_2} \qquad\qquad\qquad\qquad (8\text{-}19)$$
$$Q_{s,3,0} = K_{F,3} c_0^{N_3}$$

8.8   Fertilization

Fertilization is treated as follows. A fertilization rate in kg/ha (total surface are of flow domain) is transformed into an amount that enters each of the control volumes (CV) that are fertilized expressed in mg cm^{-3} . Not all CVs at the soil surface have to be fertilized; banded fertilization or injected fertilization is also possible. The fertilization rate dF/dt in Eq. (8-1) then follows from

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{F_A}{\Delta t} 10^{-2} \frac{A}{\displaystyle\sum_{i=1}^{n} V_i} \qquad\qquad\qquad (8\text{-}20)$$

where
F_A	fertilization rate in kg/ha total flow domain	kg ha^{-1}
Δt	time step	t
10^{-2}	conversion factor	mg kg^{-1} ha cm^{-2}
A	total surface area of flow domain	cm^2
V_i	volume of control volume i where fertilization takes place	cm^3
n	number of control volumes where fertilization takes place	-

8.9   References

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9 Non-zero sink nutrient uptake

Peter de Willigen

9.1 Non-zero sink nutrient uptake

Heinen and de Willigen (1998) considered uptake of nutrients according to the zero-sink concept of de Willigen and van Noordwijk (1987, 1994a,b). The solution of de Willigen and van Noordwijk (1987, 1994a,b) can be extended for non-zero sink conditions. The solution in dimensionless parameters is given as

$$w = -\frac{r^2 - 1}{2G}\left(\bar{c} - \bar{c}_1\right) \tag{9-1}$$

with

$$\bar{c}_1 = c_{\min}\frac{r^{2n+2} - 1}{(n+1)(r^2 - 1)} \tag{9-2}$$

With Eq. (9-2), Eq. (9-1) becomes

$$w = -\frac{r^2 - 1}{2G}\bar{c} + \frac{r^{2n+2} - 1}{(n+1)2G}c_{\min} \tag{9-3}$$

Substituting the dimensionless parameters w, and c by their respective dimension-bearing parameters (see Table 9.1 of de Willigen and van Noordwijk, 1987), and assuming no adsorption ($b = 1$), one obtains finally (cf. Eq. [50] of Heinen and de Willigen, 1998)

$$S_{sm} = p\Delta z L_{rv} D\frac{r^2 - 1}{2G}\left(\overline{C} - \frac{r^{2n+2} - 1}{(n+1)(r^2 - 1)}C_{\min}\right) \tag{9-4}$$

where

S_{sm}	maximum possible uptake rate per unit surface area of substrate	$ML^{-2}T^{-1}$
Δz	thickness of the CV layer	L
L_{rv}	root length density	LL^{-3}
D	diffusion coefficient	L^2T^{-1}
r	dimensionless reduced radius of the cylinder surrounding each root: $r = R_1/R_0$	-
G	dimensionless geometry function	-

$\boldsymbol{n}$	dimensionless water uptake by the root	-
$\overline{C}$	average concentration in the bulk substrate surrounding the root	ML^{-3}
C_{min}	minimum concentration at the root surface above which uptake can occur	ML^{-3}

For $\boldsymbol{n} < 0$ the term in front of C_{min} in Eq. (9-4) is less than 1. For example, for $\boldsymbol{n} = -0.01$, $R_0 = 0.02$ cm, this term ranges from 0.92 at $L_{rv} = 0.1$ to 0.96 at $L_{rv} = 5$.

For $\boldsymbol{n} = 0$ (diffusion only), Eq. (9-4) becomes

$$S_{sm} = \boldsymbol{p} \Delta z L_{rv} D \frac{\boldsymbol{r}^2 - 1}{2G} \left(\overline{C} - C_{min} \right) \tag{9-5}$$

For $C_{min} = 0$ (zero-sink), Eq. (9-4) becomes (Eq. [50] of Heinen and de Willigen, 1998)

$$S_{sm} = \boldsymbol{p} \Delta z L_{rv} D \frac{\boldsymbol{r}^2 - 1}{2G} \overline{C} \tag{9-6}$$

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10 Expo-linear growth and demand

Peter de Willigen and Marius Heinen

10.1 Introduction

For some situations one is not interested in coupling FUSSIM2 with an existing plant growth model, and a simple growth function suffices. Here we describe a module which is integrated in FUSSIM2 that includes an expo-linear growth equation and a nutrient demand function.

10.2 Expo-linear growth

Expo-linear growth describes growth as en exponential phase for early stages of growth which for later stages of growth turns towards linear increase in dry matter. The expo-linear growth function reads (Goudriaan and van Laar, their Eq. 2.4)

$$\frac{\mathrm{d}W_{T,p}}{\mathrm{d}t} = c_m \left(1 - \exp\left(-\frac{r_m}{c_m} W_T \right) \right) \tag{10-1}$$

where

$W_{T,p}$	potential total plant weight	kg ha^{-1}
W_T	actual total plant weight	kg ha^{-1}
t	time	d
c_m	maximum growth rate	kg ha^{-1} d^{-1}
r_m	maximum relative growth rate	kg kg^{-1} d^{-1}

In Eq. (10-1) the potential growth at given plant weight W_T is computed. The actual growth rate may be reduced, for example, due to a reduction in water uptake. Currently, only reduction to water uptake (as computed elsewhere) is implemented, so that

$$\frac{\mathrm{d}W_T}{\mathrm{d}t} = \frac{T_a}{T_p} \frac{\mathrm{d}W_{T,p}}{\mathrm{d}t} \tag{10-2}$$

where

T_p	potential water uptake	cm d^{-1}
T_a	actual water uptake	cm d^{-1}

Equations (10-1) and (10-2) are solved explicitly, so that

$$W_{T,p}^{t+\Delta t} = W_{T,p}^{t} + \frac{\mathrm{d}W_{T,p}}{\mathrm{d}t}\Delta t$$

$$W_{T}^{t+\Delta t} = W_{T}^{t} + \frac{\mathrm{d}W_{T}}{\mathrm{d}t}\Delta t$$

(10-3)

With the help of the shoot-root ratio we can compute also compute the dry matter increase in roots that can be used in the root diffusion module (see chapter 15)

$$\frac{\mathrm{d}W_{T,r}}{\mathrm{d}t} = \frac{\mathrm{d}W_{T}}{\mathrm{d}t}SHRT$$

(10-4)

where
  $SHRT$ shoot-root ratio   g g^{-1}

Additionally, the leaf area index (for example, to be used for transpiration computations) can be computed as (Goudriaan and van Laar, their Eq. 2.14)

$$LAI^{t+\Delta t} = W_{T}^{t+\Delta t}P_{L}SLA$$

(10-5)

where
  P_{L} fraction of total dry matter that are leafs   g g^{-1}
  SLA specific leaf area   ha kg^{-1}

10.3   Nutrient demand

With increase in plant mass nutrients have to be taken up as well. Here we describe the Greenwood demand function that is implemented in FUSSIM2. The Greenwood function reads (Greenwood and Draycott, 1995; their Eqs. (4), (11), (12))

$$N_O = a_G + b_G \exp(-c_G W_T)$$

(10-6)

where
  N_O optimal nutrient content in the plant   g (nutrient) g^{-1} (plant)
  a_G Greenwood a parameter   g (nutrient) g^{-1} (plant)
  b_G Greenwood b parameter   g (nutrient) g^{-1} (plant)
  c_G Greenwood c parameter   ha kg^{-1}

At any time t the actual content of the plant is known as well, e.g. it can be computed from the total uptake and the total weight

$$N_A = \frac{U}{W_T}$$

(10-7)

where

    N_A actual nutrient content in the plant   g (nutrient) g^{-1} (plant)
    U total uptake since start   kg ha^{-1}

The demand for the coming time step is computed as follows. Three pools are considered:

1) requirement due to new growth (kg ha^{-1})

$$N_{dem,1} = \frac{\mathrm{d}W_T}{\mathrm{d}t} N_O \Delta t \tag{10-8}$$

2) requirement due to change in N_O (kg ha^{-1})

$$N_{dem,2} = -W_T \frac{\mathrm{d}W_T}{\mathrm{d}t} b_G c_G \exp\left(- c_G W_T \right)\Delta t \tag{10-9}$$

where the term $b_G c_G \exp(-c_G W_T)$ is the derivative $\mathrm{d}N_O/\mathrm{d}W_T$;

3) requirement due to restore from N_A to N_O (kg ha^{-1})

$$N_{dem,3} = W_T\left(N_O - N_A\right) \tag{10-10}$$

The total demand rate N_{dem} (kg ha^{-1} d^{-1}) is computed as

$$N_{dem} = \frac{N_{dem,1} + N_{dem,2} + N_{dem,3}}{t_N} \tag{10-11}$$

where

    t_N time constant for nutrient uptake (typically 1 d)   d

Alternatively, the user may supply tabulated N_O – W_T data from which the three demand-pools and their sum can be computed similarly to Eqs. (10-8)-(10-11); of course, in Eq. (10-9) the term $b_G c_G \exp(-c_G W_T)$ is replaced by the slope belonging to the tabulated data.

10.4   References

Goudriaan J. and H.H. van Laar, 1994. Modelling potential crop growth processes. Current issues in production ecology vol. 2, Kluwer Academic Publishers, Dordrecht.

Greenwood D.J. and A. Draycott, 1995. Modelling uptake of nitrogen, phosphate and potassium in relation to crop growth. In: P. Kabat, B. Marshall, B.J. van den Broek, J. Vos and H. van Keulen, Modelling and Parameterization of the Soil-Plant-Atmosphere System. A Comparison of Potato Growth Models. Wageningen Pers, Wageningen, The Netherlands, pp. 155-175.

11 Root growth described as a diffusion process

Peter de Willigen

11.1 Diffusive root growth in two dimensions

De Willigen *et al.* (2001) postulate to describe root growth as a diffusion process. In two dimensions the root growth diffusion equation reads

$$\frac{\partial L_{rv}}{\partial t} = \frac{\partial}{\partial x}\left(D_{L,x}\frac{\partial L_{rv}}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_{L,z}\frac{\partial L_{rv}}{\partial z}\right) - \mathbf{l}_L L_{rv} + Q_L(x,z,t) \qquad (11\text{-}1)$$

where

L_{rv}	root length density	LL^{-3}
t	time	T
x	horizontal coordinate	L
z	vertical coordinate	L
$D_{L,x}$	diffusion coefficient for root growth in the x direction	L^{2}T^{-1}
$D_{L,z}$	diffusion coefficient for root growth in the z direction	L^{2}T^{-1}
$\mathbf{l}_L$	specific decay rate of roots	T^{-1}
Q_L	input rate of roots due to growth	LL^{-3}T^{-1}

De Willigen *et al.* (2001) describe all features of Eq. (11-1). Here we mention only that the one-dimensional version of Eq. (11-1) results in an exponential L_{rv} distribution with depth, which is commonly observed under non-limiting field-conditions. For the two-dimensional version of Eq. (11-1) it is obvious that for different ratios of $D_{L,x}/D_{L,z}$ different distributions with respect to horizontal or vertical growth can be obtained.

11.2 Numerical solution

Equation (11-1) is solved explicitly according to where the same notation conventions are used as in Heinen and de Willigen (1998; their section 3.2.2). The diffusion coefficients and the input rate parameters are described in the two following sections.

$$L_{rv,I,J}^{t+\Delta t} = L_{rv,I,J}^{t}$$

$$+ \left\{ \cfrac{D_{x,i} \cfrac{\left(L_{rv,I+1,J}^{t} - L_{rv,I,J}^{t}\right)}{\Delta x_i} - D_{x,i-1} \cfrac{\left(L_{rv,I,J}^{t} - L_{rv,I-1,J}^{t}\right)}{\Delta x_{i-1}}}{\Delta z_J} \right. \tag{11-2}$$

$$\left. + \cfrac{D_{z,j} \cfrac{\left(L_{rv,I,J+1}^{t} - L_{rv,I,J}^{t}\right)}{\Delta z_j} - D_{z,j-1} \cfrac{\left(L_{rv,I,J}^{t} - L_{rv,I,J-1}^{t}\right)}{\Delta z_{j-1}}}{\Delta x_I} - I_L L_{rv,I,J}^{t} + Q_{L,I,J} \right\} \Delta t$$

11.3 Diffusion coefficients

In Eq. (11-2) the diffusion coefficients at the CV interfaces are needed. They are computed as the weighted geometric average (see Heinen and de Willigen, 1998; e.g. their Eq. [63]). The diffusion coefficients of the individual CVs are in principal equal to the constant root growth diffusion coefficients in the x and z directions, $D_{L,x}$ and $D_{L,z}$, respectively. However, to simulate that growth may be hindered in extremely wet or extremely dry regions, we have implemented a reduction factor on $D_{L,x}$ and $D_{L,z}$ according to

$$\begin{aligned} D_{L,x} &= D_{L,x,0}\, f(h) \\ D_{L,z} &= D_{L,z,0}\, f(h) \end{aligned} \tag{11-3}$$

where

$D_{L,x,0}$	basic diffusion coefficient for root growth in the x direction	$L^2 T^{-1}$
$D_{L,z,0}$	basic diffusion coefficient for root growth in the z direction	$L^2 T^{-1}$
$f(h)$	reduction function	

The reduction function $f(h)$, where h is the pressure head, consist of tabulated data on h and the reduction factor $f(h)$ in the range [0,1]. The simulation program uses linear interpolation for intermediate values of h. In Table 11-1 an example of $f(h)$ is given.

Table 13-1. Example of reduction function f(h) (as used in Eq. (11-3)).

h	$f(h)$
-100000	0
-10000	0
-1000	1
-10	1
0	0
1000	0

11.4 Input rate of roots

The input rate of root length density $Q_{L,IJ}$ for each of the CVs is computed from the total input of root dry mass per time step and the location in the soil where root mass origins, i.e. mostly at the soil surface at the plant location; another location may be at a certain depth where roots originate at bulbs. So, for most CVs $Q_{L,IJ}$ will be zero as no roots originate at these CVs.

Now we only have to transform root mass input to root length input. This is done according to

$$Q_L(x,z,t) = M_r(x,z,t)\frac{1}{\mathbf{p}R_0^2\,\mathbf{r}_r\,DM_r}\frac{A}{V} \tag{11-4}$$

where

Q_L	input rate of roots due to growth	$LL^{-3}T^{-1}$
M_r	rate of dry mass input	$ML^{-2}T^{-1}$
R_0	root radius	L
$\mathbf{r}_r$	bulk density of the root	ML^{-3}
DM_r	dry matter content of root	MM^{-1}
A	surface area occupied by the plant	L^2
V	sum of volumes of all CVs where root input occurs	L^3

The parameters R_0, $\mathbf{r}_r$, DM_r, A, and V are constants, and M_r is the time-varying root input parameter that should be supplied by some plant growth model.

11.5 Fitting parameters

A fitting program is available from the authors that fits the parameters $D_{L,x,0}$, $D_{L,z,0}$, and $\mathbf{l}_L$ to measured L_{rv} profiles, e.g. as obtained from needle-boards taken from the soil.

11.6 References

De Willigen P., M. Heinen, A. Mollier and M. van Noordwijk, 2001. Two dimensional growth of a root system described as diffusion. I. Analytical solutions. *In prep.*

12   Nitrification and denitrification module NITDEN

Sjaak Conijn and Marius Heinen

12.1   Introduction

A subroutine has been added to FUSSIM2 that simulates NITrification and DENitrification (NITDEN). This subroutine was used to simulate the dynamics in conversion and production rates of ammonium and nitrate in the soil and the gaseous losses of N_2 and N_2O due to denitrification from grassland. Most of the underlying equations have been taken from Bril *et al.* (1994). Below the relevant aspects will be briefly described. The reader is referred to chapter 15 '*User's Guide*' to see the structure of the input file and some typical values and ranges for values of the parameters used below.

12.2   Nitrification

The conversion of ammonium through nitrification is given by

$$\frac{d\text{NH}_4^+}{dt} = f_{W,1}\, f_{T,1}\, f_{pH,1}\, f_{CEC}\, \frac{\text{NH}_4^+}{n_1 + \left(\dfrac{10^3\, \text{NH}_4^+}{14\, M_{ws}}\right)^2} \tag{12-1}$$

where

NH_4^+	ammonium concentration	mg cm^{-3} (soil)
t	time	d
M_{ws}	mass of wet soil	g cm^{-3} (soil)
14	molar mass of nitrogen	g mol^{-1}
10^3	conversion factor	g kg^{-1}
n_1	parameter used to calculate a multiplication factor which represents the effect of the NH_4 concentration in the soil on nitrification rate	mmol^2 kg^{-2} (wet soil)

The functional relationships f are explained below. The effect of soil water content via water filled pore space *WFPS* (-) on nitrification is given by the functional relationship $f_{W,1}$

$$f_{W,1} = \text{MAX}\left[0, \left(\sin\left(p\, WFPS^{n_2}\right)\right)^{n_3}\right] \tag{12-2}$$

where

n_2 curve shape parameter for the effect of water filled pore
           space on nitrification rate that determines the value of the
           optimum *WFPS*, where $f_{W,1} = 1$ -

n_3 curve shape parameter for the effect of water filled
           pore space on nitrification rate that determines the area underneath
           the optimum curve   -

The effect of soil temperature T (^{0}C) on nitrification is given by the functional relationship $f_{T,1}$

$$f_{T,1} = \begin{cases} 0 & T < 0 \\ \dfrac{n_4 T^{n_5}}{1 + n_6 T^{n_7}} & T \geq 0 \end{cases} \qquad (12\text{-}3)$$

where
     $n_{4,5,6,7}$ curve shape parameters   -

The effect of soil *pH* on nitrification is given by the functional relationship $f_{pH,1}$

$$f_{pH,1} = \frac{1}{1 + n_8 10^{-pH}} \qquad (12\text{-}4)$$

where
     n_8 curve shape parameter for the effect of pH on nitrification
           rate, that determines the value of the pH, where $f_{pH,1} = 0.5$ -

The effect of cation exchange capacity of the soil *CEC* (cmol$^+$ kg^{-1}) on nitrification is given by the functional relationship f_{CEC}

$$f_{CEC} = n_9 - n_{10} \log(CEC) \qquad (12\text{-}5)$$

where
     n_9 intercept of relationship between f_{CEC} and log
           (*CEC*)   mmol^2 kg^{-2} (wet soil) d^{-1}
     n_{10} slope of relationship between f_{CEC} and log
           (*CEC*)   mmol^2 kg^{-2} (wet soil) d^{-1}

Nitrification of ammonium produces not only NO_3, but also N_2O. This has been modeled by using a dimensionless partitioning factor PF_1, which is described as a function of soil *WFPS*:

$$PF_1 = \begin{cases} n_{11} & WFPS < n_{13} \\ n_{11} + n_{12} \left(\dfrac{WFPS - n_{13}}{1 - n_{13}} \right)^{n_{14}} & WFPS \geq n_{13} \end{cases} \qquad (12\text{-}6)$$

where

n_{11} minimum fraction of total nitrification that is converted into N_2O -

n_{12} maximum fraction of total nitrification that is converted into N_2O -

n_{13} *WFPS* threshold value below which the effect of *WFPS*
on N_2O production
from nitrification equals zero   -

n_{14} curve shape parameter that determines the steepness
of the curve relating the fraction converted into N_2O to *WFPS*   -

PF_1 gives the part of the total nitrification of equation 12-1 that is converted into N_2O. The production of NO_3 from nitrification is then given by the product of total nitrification and $(1 - PF_1)$.

In the above equations M_{ws}, *WFPS* and T are dynamically computed by FUSSIM2. *pH*, *CEC* and n_1 through n_{14} are all assumed constant and taken from the input file.

12.3   Denitrification

Decay of organic matter in the soil by aerobic micro-organisms requires oxygen. At low O_2 levels in the soil, the oxygen can also be provided by NO_3 and N_2O. In this process electrons are transferred from the organic matter to NO_3 and N_2O. NO_3 is then denitrified to N_2O and N_2O is denitrified to N_2. Total denitrification, expressed as total electron production accepted by either NO_3 or N_2O, is given by

$$\frac{de_p}{dt} = f_{W,2}\, f_{T,2}\, DPR \frac{\left(0.8 \dfrac{NO_3^-}{14 M_{ws}} + 0.4 \dfrac{N_2O}{28 M_{ws}} \right)}{d_1 + \left(0.8 \dfrac{NO_3^-}{14 M_{ws}} + 0.4 \dfrac{N_2O}{28 M_{ws}} \right)} \qquad (12\text{-}7)$$

where

e_p electrons produced   mmol electron cm^{-3} (soil) d^{-1}

NO_3^- nitrate concentration   mg cm^{-3} (soil)

N_2O total nitrous oxide concentration   mg cm^{-3} (soil)

DPR   potential denitrification rate of the soil   mmol electron cm^{-3} (soil) d^{-1}

14   molar mass of N   g mol^{-1}

28   = 2 * 14   g mol^{-1}

0.4   electron equivalent ratio of N_2O -

0.8   electron equivalent ratio of NO_3 -

d_1 amount of source in terms of both NO_3 and N_2O corrected
for their electron-equivalents, at which the denitrification rate
equals half its maximum rate at optimal conditions for
denitrification (the half-value constant
in a Monod function)   mol N kg^{-1} (wet soil)

DPR is defined as the maximum denitrification at a reference temperature of $20\ ^0$C in the absence of O_2 and unlimited supply of NO_3. It is thus strongly related to the decomposition rate of organic matter in the soil. Via a small adaptation of NITDEN CO_2 production from a module that simulates organic matter decay can be used instead of *DPR*. The dynamics in the soil organic matter, e.g. by using organic fertilizers, then also determines the denitrification rates.

The effect of soil water content via water filled pore space *WFPS* (-) on total denitrification is given by the functional relationship $f_{W,2}$

$$f_{W,2} = \begin{cases} 0 & WFPS < d_2 \\ \left(\dfrac{WFPS - d_2}{1 - d_2}\right)^{d_3} & WFPS \geq d_2 \end{cases}$$

(12-8)

where

d_2	*WFPS* threshold value below which the denitrification rate equals zero	-
d_3	curve shape parameter that determines the steepness of the curve for the effect of *WFPS* on denitrification rate	-

The effect of soil temperature T (^{0}C) on total denitrification is given by the functional relationship $f_{T,2}$

$$f_{T,2} = \begin{cases} 0 & T < 0 \\ \dfrac{d_4 T^{d_5}}{\left(1 + d_6 T^{d_7}\right) f_{T=20,2}} & T \geq 0 \end{cases}$$

(12-9)

where

$d_{4,5,6,7}$	curve shape parameters	-

In the denitrifcation process NO_3 and N_2O compete for the electrons produced during decay of organic matter. Reduction of NO_3 is given by

$$\frac{dNO_3^-}{dt} = \frac{NO_3^-}{\left(\dfrac{4NO_3^-}{14} + \dfrac{2N_2O}{28} d_8 f_{pH,2}\right)} \frac{de_p}{dt}$$

(12-10)

where

2	electron equivalent ratio of N_2O	-
4	electron equivalent ratio of NO_3	-
d_8	parameter that accounts for the sink strength of N_2O in consuming electrons relative to that of NO_3	-

and reduction of N_2O is given by

$$\left(\frac{dN_2O}{dt}\right)_R = \frac{N_2O\, d_8\, f_{pH,2}}{\left(\dfrac{4NO_3^-}{14} + \dfrac{2N_2O}{28}\, d_8\, f_{pH,2}\right)}\frac{de_p}{dt} \qquad (12\text{-}11)$$

The effect of soil pH on reduction of NO_3 and N_2O is given by the functional relationship $f_{pH,2}$

$$f_{pH,2} = MAX\left[d_{11}, 10^{\frac{pH-d_9}{d_{10}}}\right] \qquad (12\text{-}12)$$

where
d_9	pH value at which the factor for the sink strength of N_2O in consuming electrons relative to that of NO_3 equals d_8	-
d_{10}	curve shape parameter	-
d_{11}	minimum value for the multiplication factor for the effect of pH on the sink strength of N_2O in consuming electrons relative to that of NO_3	-

The N_2O production from denitrification of NO_3 is given by dNO_3/dt and the N_2 production equals $(dN_2O/dt)_R$.

In the above equations M_{ws}, $WFPS$ and T are used as in the equations for nitrification. DPR, pH and d_1 through d_{11} are all assumed constant and taken from the input file.

12.4 N₂O emission

As gas transport is not modelled, emission of N_2O from the soil surface towards the atmosphere is estimated as follows

$$\left(\frac{dN_2O}{dt}\right)_E = EF\left(\frac{\left(1-WFPS^{e_1}\right)}{f_a}N_2O - N_2O_{air}\right) \qquad (12\text{-}13)$$

where
N_2O_{air}	N_2O concentration of the atmosphere	mg cm³ (air)
f_a	volumetric gas content	cm³ cm⁻³ (soil)
e_1	parameter used in calculating the N_2O concentration in soil air by partitioning of total N_2O between soil water and soil air as a function of water filled pore space	-

No intrusion from atmosphere to the soil has been considered in NITDEN. The emission factor EF (d^{-1}) is given by a sigmoidal function

$$EF = \frac{e_4}{1 + \left(\dfrac{WFPS}{e_2}\right)^{e_3}} \qquad (12\text{-}14)$$

where
e_2	$WFPS$ at which EF equals half of its maximum value e_4	-
e_3	curve shape parameter for the function relating EF to $WFPS$	-
e_4	maximum fraction of the difference in N_2O concentration between soil air and atmosphere that leaves the soil as N_2O emission at $WFPS = 0$	d^{-1}

f_a and $WFPS$ are dynamically computed by FUSSIM2. N_2O_{air} and e_1 through e_4 are all assumed constant and taken from the input file.

12.5 N₂O dynamics in the soil

The governing N_2O equation describes the net N_2O rate of change in the soil as the sum of two N_2O production processes minus the sum of two N_2O consumption processes. The production processes are nitrification of NH_4 to N_2O and reduction of NO_3 to N_2O, and the two consumption processes are N_2O reduction to N_2 and N_2O emission. The governing equation reads

$$\underbrace{\frac{dN_2O}{dt}}_{\text{net } N_2O \text{ production}} = \underbrace{PF_1 \frac{dNH_4^+}{dt}}_{\text{nitrification}} + \underbrace{\frac{dNO_3^-}{dt}}_{NO_3 \text{ reduction}} - \underbrace{\left(\frac{dN_2O}{dt}\right)_R}_{N_2O \text{ reduction}} - \underbrace{\left(\frac{dN_2O}{dt}\right)_E}_{N_2O \text{ emission}} \qquad (12\text{-}15)$$

12.6 Numerical solution

Equation (12-15) is solved numerically using a semi-implicit Euler scheme. Our experience is that using explicit Euler resulted in very small time-step requirements. The semi-implicit Euler scheme reads (Press *et al*, 1992; their Eq. (16.6.17))

$$y^{t+\Delta t} = y^t + \frac{\Delta t \dfrac{dy^t}{dt}}{1 - \Delta t \dfrac{dy^t/dt}{dy^t}} \qquad (12\text{-}16)$$

The derivative dy/dt is computed according to Eqs. (12-1)-(12-15), where y represents the N$_2$O concentration in the soil. The derivative of dy/dt to y is numerically estimated by computing dy/dt for two values of N$_2$O, one somewhat less than current N$_2$O and one somewhat larger than current N$_2$O:

$$\frac{\mathrm{d}y^t/\mathrm{d}t}{\mathrm{d}y^t} = \frac{(\mathrm{d}y/\mathrm{d}t)\big|_{\mathrm{N_2O}(1+a)} - (\mathrm{d}y/\mathrm{d}t)\big|_{\mathrm{N_2O}(1-a)}}{2a\mathrm{N_2O}} \tag{12-17}$$

A typical value for α equals 0.01.

12.7 The input file NITDENIN.DAT

In chapter 15 (section 15.4.17) an example of the input file NITDENIN.DAT is presented. Here we indicate which parameter of the Eqs. (12-1) through (12-14) corresponds to which variable in this file (Table 12-1).

Table 12-1 Correspondence between variables used in text and the parameter names as occurring in the data file NITDENIN.DAT. For completeness, the units of the variables are given as well.

Variable in text	Name in NITDENIN.DAT	Units	Variable in text	Name in NITDENIN.DAT	Units
n_1	NitSourceParam1	mmol^2 kg^{-2} (wet soil)	d_1	DenSourceParam1	mol kg^{-1} (wet soil)
n_2	NitWaterParam1	-	d_2	DenWaterParam1	-
n_3	NitWaterParam2	-	d_3	DenWaterParam2	-
n_4	NitTempParam1	-	d_4	DenTempParam1	-
n_5	NitTempParam2	-	d_5	DenTempParam2	-
n_6	NitTempParam3	-	d_6	DenTempParam3	-
n_7	NitTempParam4	-	d_7	DenTempParam4	-
n_8	NitpHParam1	-	d_8	DenElectrParam1	-
n_9	NitCECParam1	mmol^2 kg^{-2} (wet soil) d^{-1}	d_9	DenpHParam1	-
n_{10}	NitCECParam2	mmol^2 kg^{-2} (wet soil) d^{-1}	d_{10}	DenpHParam2	-
n_{11}	NitPartParam1	-	d_{11}	DenpHParam3	-
n_{12}	NitPartParam2	-	e_1	DenEmisParam4	-
n_{13}	NitPartParam3	-	e_2	DenEmisParam1	-
n_{14}	NitPartParam4	-	e_3	DenEmisParam2	-
			e_4	DenEmisParam3	d^{-1}

12.8 Acknowledgements

12.9 References

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Press W.H., S.A. Teukolsky, W.T. Vetterling and B.P. Flannery, 1992. Numerical recipes in Fortran 77. Second edition. The art of scientific computing. Cambridge University Press.

13 Soil temperature (1-D)

Marius Heinen

13.1 Introduction

Soil temperature is one of the key parameters in nitrogen mineralization and (de)nitrification. Therefore, it is decided to include soil temperature dynamics in FUSSIM2. For simplicity, we consider here one-dimensional temperature profiles in the soil.

13.2 Heat conduction

The governing equation for heat conduction is given by

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(D_h \frac{\partial T}{\partial z}\right)$$

(13-1)

where

T	temperature	^0C
t	time	d
z	vertical coordinate	cm
D_h	heat diffusivity	$cm^2\ d^{-1}$

D_h is the ratio of the heat conductivity k_h (J cm^{-1} d^{-1} $^0C^{-1}$) and the volumetric heat capacity C_h (J cm^{-3} $^0C^{-1}$)

$$D_h = \frac{k_h}{C_h}$$

(13-2)

The properties C_h, k_h, and D_h are not constant, but depend on the composition of the porous medium; this will be discussed in a separate section below.

13.2.1 Integration of the heat conduction equation

Equation (13-1) is solved numerically, analogously to the solution of the water movement equation in FUSSIM2; details of the solution procedure can be found in Heinen and de Willigen (1998). The left hand side of Eq. (13-1) is approximated by

$$\int_{x}^{x+\Delta x}\int_{y}^{y+\Delta y}\int_{z_{j-1}}^{z_j}\int_{t}^{t+\Delta t}\frac{\partial T}{\partial t}\mathrm{d}t\mathrm{d}z\mathrm{d}y\mathrm{d}x = \left[T_J^{t+\Delta t} - T_J^{t}\right]\Delta x\Delta y\Delta z_J \tag{13-3}$$

The right hand side of Eq. (13-1) is approximated by

$$\int_{x}^{x+\Delta x}\int_{y}^{y+\Delta y}\int_{z_{j-1}}^{z_j}\int_{t}^{t+\Delta t}\frac{\partial}{\partial t}\left(D_h\frac{\partial T}{\partial t}\right)\mathrm{d}t\mathrm{d}z\mathrm{d}y\mathrm{d}x = \left[D_h\frac{\partial T}{\partial t}\right]_{z_{j-1}}^{z_j}\Delta x\Delta y\Delta t$$

$$= \left[D_{h,z_j}\frac{\partial T}{\partial t}\bigg|_{z_j} - D_{h,z_{j-1}}\frac{\partial T}{\partial t}\bigg|_{z_{j-1}}\right]\Delta x\Delta y\Delta t \tag{13-4}$$

$$= \left[D_{h,z_j}\frac{T_{J+1}^{t+\Delta t} - T_J^{t+\Delta t}}{\Delta z_j} - D_{h,z_{j-1}}\frac{T_J^{t+\Delta t} - T_{J-1}^{t+\Delta t}}{\Delta z_{j-1}}\right]\Delta x\Delta y\Delta t$$

The heat diffusivities at the control volume (CV) boundaries are obtained from the D_h values at the grid points through geometric averaging

$$D_{h,z_j} = D_J^{1-w}D_{J+1}^{w}$$
$$D_{h,z_{j-1}} = D_{J-1}^{1-w}D_J^{w} \tag{13-5}$$

The distance between the grid points is given by

$$\Delta z_j = \left(\Delta z_J + \Delta z_{J+1}\right)/2$$
$$\Delta z_{j-1} = \left(\Delta z_{J-1} + \Delta z_J\right)/2 \tag{13-6}$$

Rearranging gives the following approximation of Eq. (13-1)

$$A_J T_J^{t+\Delta t} - A_{S,J}T_{J+1}^{t+\Delta t} - A_{N,J}T_{J-1}^{t+\Delta t} = b_J \tag{13-7}$$

where

$$A_J = A_{S,J} + A_{N,J} + \frac{\Delta x\Delta y\Delta z_J}{\Delta t} \tag{13-8}$$

and

$$A_{S,J} = D_{h,z_j}\frac{\Delta x\Delta y}{\Delta z_j}$$

$$A_{N,J} = D_{h,z_{j-1}}\frac{\Delta x\Delta y}{\Delta z_{j-1}} \tag{13-9}$$

and

$$b_J = \frac{\Delta x \Delta y \Delta z_J}{\Delta t} T_J^t \tag{13-10}$$

Setting-up Eq. (13-7) for all CV's yields a matrix problem

$$\mathbf{A} T = b \tag{13-11}$$

For the current one-dimensional problem the coefficient matrix **A** is a three-banded matrix. The solution of Eq. (13-11) can be simply obtained using the Thomas Algorithm.

13.2.2 Boundary condition

We use only Dirichlet boundary conditions at the soil surface and at great depth. At the soil surface we set $T = T_{air}$ and at great depth we set T equal to the yearly average at that depth. The Dirichlet condition is modeled as follows. The solution given above is used, but the A and b parameters are given by

$$b_J = LT_b$$
$$A_J = L \tag{13-12}$$

where L is some large number, e.g. $L = 10^{25}$. Since A and b are so much larger than the other parameters, the solution will yield $T = T_b$, where T_b is the prescribed temperature at the boundary.

13.3   Verification

The solution procedure is verified by comparing simulated temperature profiles with analytical solutions.

13.3.1 Case 1

The transient temperature distribution in a finite cylinder with unit initial T, zero T at the boundaries and constant D_h is given by (Carslaw and Jaeger, 1959; see also example 6.1 of Heinen and de Willigen, 1998)

$$T(z,t) = \frac{4}{\boldsymbol{p}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \exp\left(-D_h \frac{(2n+1)^2 \boldsymbol{p}^2}{Z^2} t\right) \cos\left(\frac{(2n+1)\boldsymbol{p}}{Z} z\right) \tag{13-13}$$

where Z is the length of the cylinder.

Figure 13-1 shows the comparison between simulated (using constant $\Delta t = 10^{-3}$ d) and analytical solutions. In Table 13-1 the difference (sum of squared differences) between simulated and analytical solutions is given for different time steps used in the numerical solution procedure. Parameters used: 20 layers of unit thickness, $D_h = 724.11 \text{ cm}^2 \text{ d}^{-1}$.
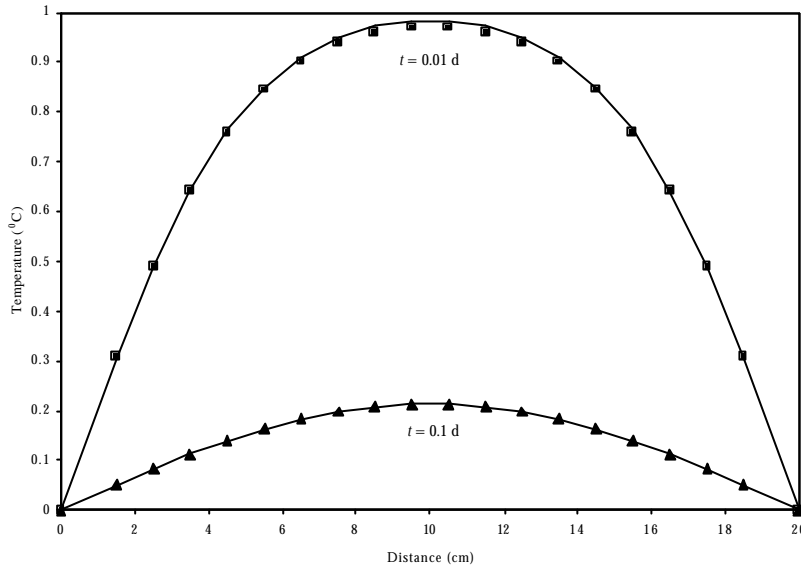
Figure 13-1. Comparison between simulated (markers) and analytical (lines) temperature profiles for case 1 at two times.

Table 13-1. Sum of squared differences (SSQ) between simulated and analytical solutions at times t = 0.1 and 0.01 d for case 1. Different time steps $\mathbf{D}t$ were used: constant ($\mathbf{D}t = \mathbf{D}t_{max}$) or gradually increasing time steps ($\mathbf{D}t < \mathbf{D}t_{max}$) in which case $\mathbf{D}t$ was gradually increased by a factor 1.1 until maximum allowable time step $\mathbf{D}t_{max}$ was reached.

Δt	Δt_{max}	SSQ, $t = 0.1$ d	SSQ, $t = 0.01$ d
10^{-1}	10^{-1}	$5.8\ 10^{-1}$	n.a.
10^{-2}	10^{-2}	$9.3\ 10^{-3}$	$5.5\ 10^{-2}$
10^{-3}	10^{-3}	$2.2\ 10^{-5}$	$8.9\ 10^{-4}$
10^{-4}	10^{-4}	$2.4\ 10^{-5}$	$1.3\ 10^{-3}$
10^{-5}	10^{-5}	$3.4\ 10^{-5}$	$1.5\ 10^{-3}$
10^{-6}	10^{-6}	$3.5\ 10^{-5}$	$1.5\ 10^{-3}$
10^{-2}	10^{-1}	$1.7\ 10^{-2}$	n.a.
10^{-3}	10^{-2}	$2.6\ 10^{-3}$	$1.1\ 10^{-3}$
10^{-4}	10^{-3}	$1.8\ 10^{-5}$	$9.1\ 10^{-4}$
10^{-5}	10^{-4}	$2.4\ 10^{-5}$	$1.4\ 10^{-3}$
10^{-6}	10^{-5}	$3.4\ 10^{-5}$	$1.5\ 10^{-3}$
10^{-6}	10^{-3}	$1.7\ 10^{-5}$	$9.7\ 10^{-4}$

13.3.2 Case 2

The transient temperature distribution in a finite cylinder with a parabolic initial T distribution, zero T at the boundaries, unit T at the center of the cylinder, and constant D_h is given by (Carslaw and Jaeger, 1959; see also example 6.1 of Heinen and de Willigen, 1998)

$$T(z,t) = \frac{4}{p} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \exp\left(-D_h \frac{(2n+1)^2 p^2}{Z^2} t\right) \cos\left(\frac{(2n+1)p}{Z} z\right) \qquad (13\text{-}14)$$

The initial T distribution is given by

$$T(z) = \frac{(Z/2)^2 - (z - Z/2)^2}{(Z/2)^2} \qquad (13\text{-}15)$$

Figure 13-2 shows the comparison between simulated (using constant $\Delta t = 10^{-3}$ d) and analytical solutions. In Table 13-2 the difference (sum of squared differences) between simulated and analytical solutions is given for different time steps used in the numerical solution procedure. Parameters used: 20 layers of unit thickness, $D_h = 724.11$ cm^2 d^{-1}.
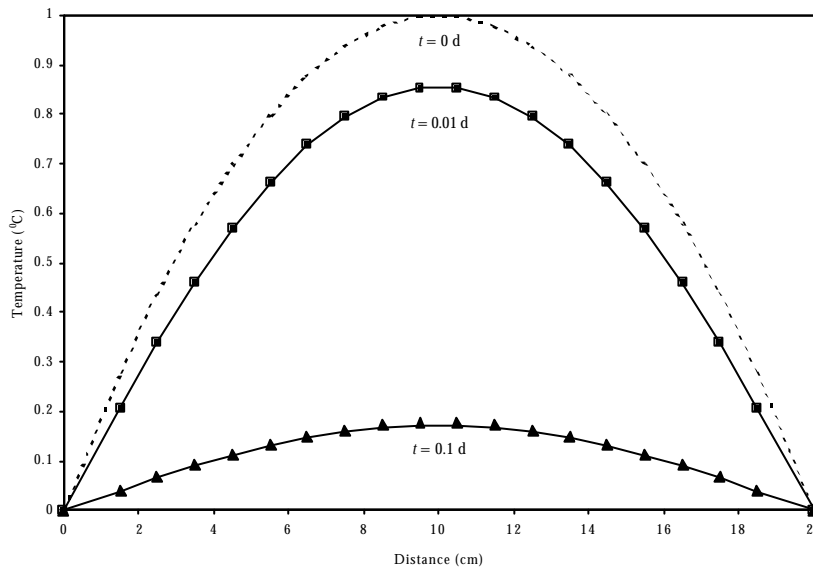
Figure 13-2. Comparison between simulated (markers) and analytical (lines) temperature profiles for case 2 at two times.

Table 13-2. Sum of squared differences (SSQ) between simulated and analytical solutions at times t = 0.1 and 0.01 d for case 2. Different time steps $\boldsymbol{D}t$ were used: constant ($\boldsymbol{D}t = \boldsymbol{D}t_{max}$) or gradually increasing time steps ($\boldsymbol{D}t < \boldsymbol{D}t_{max}$) in which case $\boldsymbol{D}t$ was gradually increased by a factor 1.1 until maximum allowable time step $\boldsymbol{D}t_{max}$ was reached.

Δt	Δt_{max}	SSQ, $t = 0.1$ d	SSQ, $t = 0.01$ d
10^{-1}	10^{-1}	3.9×10^{-1}	n.a.
10^{-2}	10^{-2}	7.1×10^{-3}	2.0×10^{-3}
10^{-3}	10^{-3}	8.8×10^{-5}	2.2×10^{-5}
10^{-4}	10^{-4}	2.5×10^{-6}	1.0×10^{-6}
10^{-5}	10^{-5}	6.5×10^{-7}	1.4×10^{-6}
10^{-6}	10^{-6}	5.4×10^{-7}	1.5×10^{-6}
10^{-2}	10^{-1}	1.3×10^{-2}	n.a.
10^{-3}	10^{-2}	2.3×10^{-3}	4.2×10^{-5}
10^{-4}	10^{-3}	8.1×10^{-5}	6.1×10^{-6}
10^{-5}	10^{-4}	2.4×10^{-6}	1.0×10^{-6}
10^{-6}	10^{-5}	6.5×10^{-7}	1.4×10^{-6}
10^{-6}	10^{-3}	7.9×10^{-5}	4.0×10^{-6}

13.3.3 Case 3

Although the changes in soil temperature do follow regular patterns, it is instructive to consider oscillating patterns; there are daily and annual cyclic patterns. We assume that at all depths in the soil T oscillates as a pure harmonic (sinusoidal) function of time around an average value. Despite T varies differently at different depths, we assume that at all depths the average T is the same, T_{av}. At the soil surface we assume a periodic (sinusoidal) variation of T with amplitude A_0 and radial frequency $\boldsymbol{w}$, and at infinite depth T is constant and equal to T_{av}. Under these circumstances Eq. (13-1) can be solved to yield (Koorevaar *et al.*, 1983; Hillel, 1980)

$$T(z,t) = T_{av} + A_0 e^{-z/d} \sin(\boldsymbol{w}t - z/d) \tag{13-16}$$

where d is the damping depth defined as

$$d = \sqrt{\frac{2k_h}{\boldsymbol{w}C_h}} = \sqrt{\frac{2D_h}{\boldsymbol{w}}} \tag{13-17}$$

The radial frequency $\boldsymbol{w}$ is given as

$$\boldsymbol{w} = \frac{2\boldsymbol{p}}{t_c} \tag{13-18}$$

where t_c is the time needed to complete one cycle of the harmonic wave. Equation (13-16) is rewritten, such that $T = T_{av}$ at day t_{av} yielding

$$T(z,t) = T_{av} + A_0 e^{-z/d} \sin(\boldsymbol{w}(t - t_{av}) - z/d) \tag{13-19}$$

We used Eq. (13-19) analytical solution and compared it with simulated T profiles. We considered 1 year, i.e. $t_c = 365$ d, $t_{av} = 121$ (may 1st), $T_{av} = 11.4$ ^{0}C, $A_0 = 8.4$ ^{0}C, and a sand soil at (constant) 50% saturation with $k_h = 1524.1$ J cm^{-1} d^{-1} ^{0}C^{-1} and $C_h = 2.1$ J cm^{-3} ^{0}C^{-1}. We considered a soil profile of 100 cm deep, divided in 20 layers of equal thickness. As boundary conditions for the simulation model we used T as computed from Eq. (13-19) at depths $z = 0$ and $z = 100$ cm. The simulation model used time steps of 1 d, which resulted in good comparison with the analytical solution (Figure 13-3). Note that for this particular example d (annual) $= 290$ cm, and the phase shift at depth z is given by $z/(dw)$; for example at $z = 100$ cm the phase shift is 20 d.
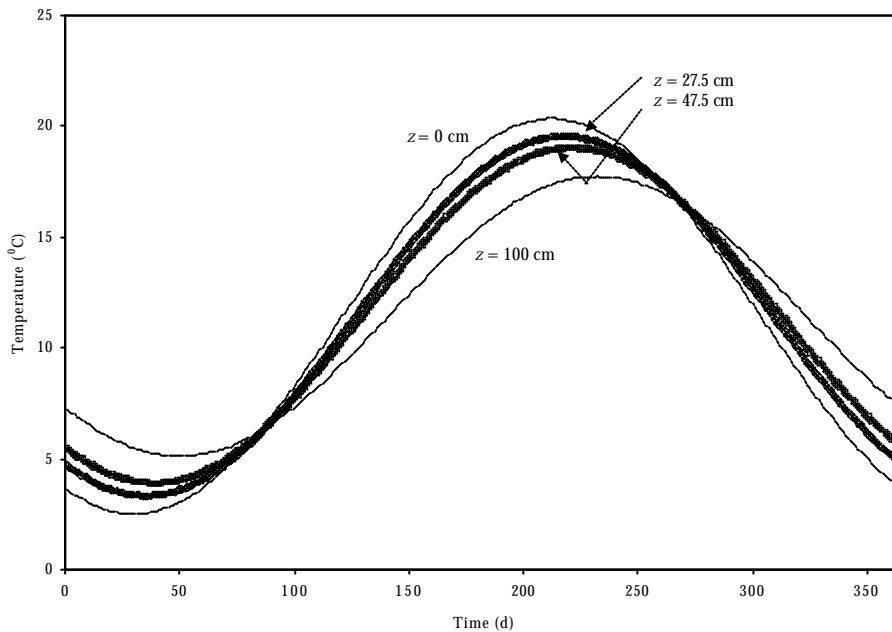
Figure 13-3. Simulated and analytical temperature profiles for case 3.

13.4 On k_h, C_h and D_h

The thermal properties k_h, C_h, and thus D_h are dependent on the composition of the porous medium (Koorevaar *et al.*, 1983; Hillel, 1980).

C_h is defied as the change in heat content of a unit bulk volume of soil per unit change in temperature (J cm^{-3} ^{0}C^{-1}). C_h depends on the composition of the soil's solid phase (the mineral and organic constituents), bulk density, and the volumetric water content. It can be calculated as the sum of the heat capacities of the various components, weighted according to their volume fractions

$$C_h = f_m C_m + f_o C_o + q C_w \qquad (13-20)$$

where

f_m	volume fraction of minerals	$cm^3\ cm^{-3}$
f_o	volume fraction of organic matter	$cm^3\ cm^{-3}$
q	volumetric water content	$cm^3\ cm^{-3}$
C_m	heat capacity of minerals	$J\ cm^{-3}\ {}^0C^{-1}$
C_o	heat capacity of organic matter	$J\ cm^{-3}\ {}^0C^{-1}$
C_w	heat capacity of water	$J\ cm^{-3}\ {}^0C^{-1}$

The contribution of air is disregarded, since it's density is much lower than that of water. Note that $f_m + f_o + q = 1 - f_a$, with f_a is the volume fraction of air. Values for the different C's are listed in Table 13-3.

Table 13-3. Densities, thermal conductivities and heat capacities of different soil constituents (from Hillel, 1980, his Tables 12.1+12.2).

Constituent	Density (kg m^{-3})	Thermal conductivity k_h (J cm^{-1} d^{-1} ^{0}C^{-1})	Heat capacity C_h (J cm^{-3} ^{0}C^{-1})
Quartz	2660	7603.2	2.0
Other minerals (average)	2650	2505.6	2.0
Organic matter	1300	216.0	2.5
Water	1000	492.5	4.2
Air	1.25	21.6	0.00125

k_h is defined as the amount of heat transferred through a unit area in unit time under a unit temperature gradient. k_h depends on the soil's mineral composition and organic matter content as well as on the volume fractions of water and air (Table 13-3 gives k_h of different components). Since the water and air content vary with time, k_h varies with time. The variation in k_h is much greater than that of C_h; under field conditions C_h may change three- or fourfold, while k_h may change a hundredfold or more. Since k_h depends on size, shape and arrangement of the soil particles, it is difficult to compute k_h of a soil. We propose to determine k_h from tabulated data for different soil types. Van Wijk and de Vries (1963; quoted by Hillel, 1980) gave the data as presented in Table 13-4 (see also Figure 13-4).

Table 13-4. Average thermal properties for three soil types (after van Wijk and de Vries (1963) as quoted by Hillel in his Table 12.3).

Soil type	Porosity (cm^3 cm^{-3})	Volumetric water content (cm^3 cm^{-3})	Degree of saturation (-)	Thermal conductivity k_h (J cm^{-1} d^{-1} K^{-1})	Heat capacity C_h (J cm^{-3} K^{-1})
Sand	0.4	0.0	0.0	254.0	1.26
	0.4	0.2	0.5	1524.1	2.10
	0.4	0.4	1.0	1887.0	2.94
Clay	0.4	0.0	0.0	217.7	1.26
	0.4	0.2	0.5	1016.1	2.10
	0.4	0.4	1.0	1378.9	2.94
Peat	0.8	0.0	0.0	50.8	1.47
	0.8	0.4	0.5	254.0	3.15
	0.8	0.8	1.0	435.5	4.83
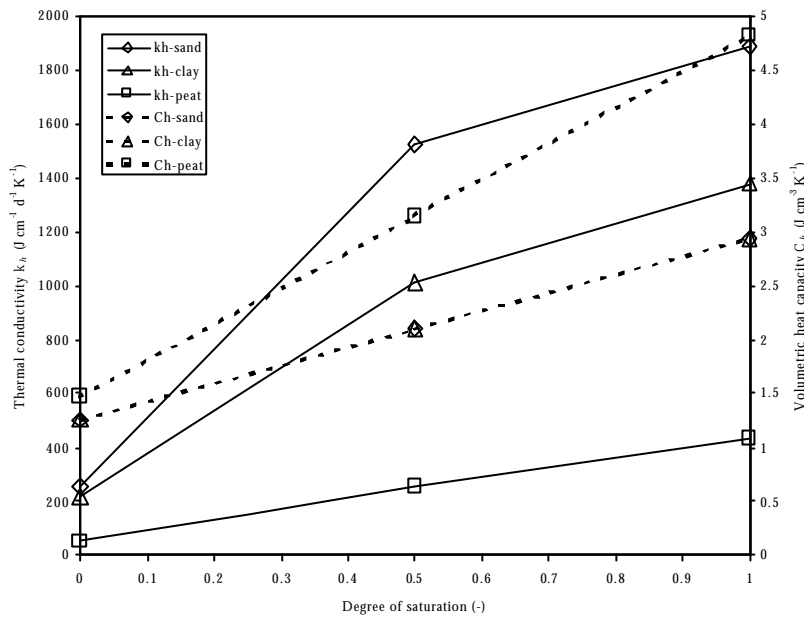
Figure 13-4. Average thermal properties for three soil types as given in Table 13-4.

13.5 Implementation in FUSSIM2

The 1-D heat conduction equation is solved numerically according to Eqs. (13-7) - (13-12) using the Thomas Algorithm. The boundary condition at the soil surface can be either computed from Eq. (13-19) or be set equal to the average day temperature of the air (the average of measured minimum and maximum daily air temperature from meteorological data files). At the bottom of the soil profile the boundary condition is the temperature as computed from Eq.(13-19).

The thermal properties are computed s follows. For each soil layer C_h can be computed according to Eq.(13-20), or be linearly interpolated from data of Table 13-4. In the first case the dry bulk density r_d (kg m^{-3}) of the soil layer and the organic matter volume fraction f_o (cm^3 cm^{-3}) must be known. From these two data the volume fraction of the minerals f_m (cm^3 cm^{-3}) is computed as in which r_o and r_m are known from Table 13-3. Then for given q, C_h can be computed from Eq. (13-20). In the second case, for each soil layer it must be indicated if it is a sand, a clay or a peat layer, and the porosity f (cm^3 cm^{-3}) must be supplied. Then for given q, the degree of saturation is given by q/f and C_h can be obtained through linear interpolation from Table 13-4.

$$f_m = \frac{r_d - r_o f_o}{r_m} \tag{13-21}$$

For k_h the second method of computing C_h is applied, i.e. the user supplies type of soil (sand, clay or peat) per layer and its porosity. At given $\mathbf{q}$, k_h is obtained through linear interpolation from data of Table 13-4).

The thermal diffusivity D_h of each layer is computed from C_h and k_h according to Eq. (13-2).

The top boundary condition is either computed from Eq. (13-19) or can be supplied by the user in the main module that is calling the routine STEMP. For example, the user may know any measured soil surface temperature, or may supply the average day temperature of the air. For the bottom boundary condition the choice exists as for the top boundary condition.

The main parameters needed by the routine STEMP should be supplied in a data file with the name STEMP.DAT, as described in chapter 16.

13.6   References

Carslaw H.S. and J.C. Jaeger, 1959. Conduction of heat in solids, 2nd edition. Clarendon Press, Oxford.

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14 Coupling with MOTOR

Peter de Willigen and Marius Heinen

14.1 Introduction

Solute transport of N in soil (or substrate) is described by a continuity equation. In such an equation sources and sinks must be considered, such as root uptake and sources or sinks due to organic matter dynamics. In this chapter we describe how the model FUSSIM2 (Heinen and de Willigen, 1998) and the model MOTOR (Rappoldt, 2001; Whitmore, 1995) are combined. The model FUSSIM2 describes water movement, solute transport and root uptake of water and solutes. The model MOTOR is a MOdule describing the Transformation of Organic matteR and nutrients in soil. We used the FSE version of Rappoldt (2001) which is totally based on the concepts of Whitmore (1995). Both versions of MOTOR produce identical results (Rappoldt, pers. comm.).

In this chapter we shortly describe how MOTOR is incorporated in FUSSIM2. Secondly we present an analytical solution for a set of transformations in order to verify the numerical solution of MOTOR.

14.2 Incorporation of MOTOR in FUSSIM2

The MOTOR version of Rappoldt (2001) is a stand-alone model. The computations are governed by a Runge-Kutta driver. For the incorporation in FUSSIM2 it was decided to retain as much as possible all statement of the driver and the model. The Runge-Kutta driver was changed such that it could be called from outside (i.e. from FUSSIM2) with four different tasks: initialization, dynamic, output, and terminal. Furthermore, it was essential that for several layers (or control volumes) in FUSSIM2 different transformation can be handled. In other words the states of MOTOR in the driver and the model must be stored. Storage is done in arrays, which are finally stored per layer (or control volume) in FUSSIM2. There are two ways of storage: a simple storage of the states only, and a complete storage of all model variables. The second method is the most flexible, but costs a large amount of memory storage (and some more computational time). The first method can only be used if for all layers considered the same transformations are used, the same transformation tables, etc., with the only difference the initial distribution of the pools.

Other changes to the driver are: no regular output governed by the driver other than output during state and time events, time (begin and end of the simulation interval) is governed by the calling routine FUSSIM2, and the water content and temperature correction data come from the calling routine FUSSIM2.

14.3   Analytical solution to verify MOTOR

The numerical solution of the model MOTOR can be verified against an analytical solution. First we present the general procedure how an analytical solution can be obtained. Secondly, we present a comparison of the numerical and analytical solution for a simple example.

An analytical solution is presented for first-order kinetics. For N pools there are at maximum NxN transformations possible, but generally much less than NxN transformations occur. In general, the transformation of pool y_i is described by

$$\frac{dy_i}{dt} = e_{i,1}k_{i,1}\,y_1 + ... - k_i\,y_i + ... + e_{i,n}k_{i,n}\,y_n \tag{14-1}$$

where
y	pool	ML^{-2} or MM^{-1}
k	rate constant	T^{-1}
e	efficiency parameter in the range [0,1]	

Pool y_i increases due to production (+) from other pools, and decreases (-) due to transformation of y_i into another pool. Equation (14-1) can be set up for all N pools. The resulting set of equations can be represented by the following matrix problem

$$\frac{d\mathbf{y}}{dt} = \mathbf{k} \cdot \mathbf{y} \tag{14-2}$$

where $\mathbf{y}$ is the vector with the N pools, and $\mathbf{k}$ is the coefficient matrix, which for, e.g., N=3 has the form

$$\mathbf{k} = \begin{pmatrix} -k_1 & k_{2,1}e_{2,1} & k_{3,1}e_{3,1} \\ k_{1,2}e_{1,2} & -k_2 & k_{3,2}e_{3,2} \\ k_{1,3}e_{1,3} & k_{2,3}e_{2,3} & -k_3 \end{pmatrix} \tag{14-3}$$

Equation (14-2) can be solved using Laplace transformation. The Laplace transformed version of Eq. (14-2) reads

$$s\mathbf{I} \cdot \mathbf{U} - \mathbf{y}_0 = \mathbf{k} \cdot \mathbf{U} \tag{14-4}$$

where
s	the Laplace parameter
$\mathbf{I}$	the NxN identity matrix
$\mathbf{U}$	the Laplace transformed y vector
$\mathbf{y}_0$	the vector with initial y values.

Equation (14-4) can be solved for **U** and the final solution **y** is obtained via the Laplace back-transformation: $\mathbf{y} = \Lambda^{-1}(\mathbf{U})$.

$$\mathbf{U} = (s\mathbf{I} - \mathbf{k})^{-1} \cdot \mathbf{y}_0 \qquad (14\text{-}5)$$

We now consider an example for $N = 5$ with 8 transformations. The data are given in Table 14-1. The five pools are, respectively, biomass, active organic matter (ActiveOM), physically protected organic matter (PhysPOM), chemically protected organic matter (ChemPOM), and physically-chemically protected organic matter (PhChPOM). The coefficient matrix **k** in this case reads (the columns represent the sources, and the rows represent the produce)

$$\mathbf{k} = \begin{pmatrix} -8\ 10^{-3} & 1.2\ 10^{-2} & 0 & 1.2\ 10^{-6} & 0 \\ 6\ 10^{-3} & -3.5\ 10^{-2} & 1.5\ 10^{-3} & 0 & 0 \\ 0 & 1.5\ 10^{-2} & -1.5\ 10^{-3} & 0 & 0 \\ 1.2\ 10^{-3} & 0 & 0 & -15.002\ 10^{-2} & 1.5\ 10^{-3} \\ 0 & 0 & 0 & 1.5\ 10^{-2} & -1.5\ 10^{-3} \end{pmatrix} \qquad (14\text{-}6)$$

*Table 14-1. Transformation table for 5 pools of substrate indicating the produce, rate constant k (d^{-1}), and the efficiency **e** (-).*

Substrate	Produce	k	e
Biomass	ActiveOM	6.0 10^{-3}	1.0
Biomass	ChemPOM	2.0 10^{-3}	0.6
ActiveOM	Biomass	2.0 10^{-2}	0.6
PhysPOM	ActiveOM	1.5 10^{-3}	1.0
ChemPOM	Biomass	2.0 10^{-6}	0.6
PhChPOM	ChemPOM	1.5 10^{-3}	1.0
ActiveOM	PhysPOM	1.5 10^{-2}	1.0
ChemPOM	PhChPOM	1.5 10^{-2}	1.0

The solution of Eq. (14-5), i.e. **U**, and the final solution **y** were obtained using Mathematica (Wolfram, 1991). Figure 14-1 presents the excellent comparison between the numerically obtained (using FUSSIM2+MOTOR) and analytical solutions for the change of the five pools as a function of time. The results pertain to the carbon-fraction of the pools, with $\mathbf{y}_0 = \{100, 100, 1000, 4500, 12000\}$ (kg ha^{-1}). It was taken care in the numerical model that ample nitrogen was available to let the transformations continue at the maximum rates.

Generally, the transformations are influenced by other external conditions, which in the example above were taken as optimal. The model MOTOR uses water content and temperature reductions on the rate constants, which, if constant, can be simple incorporated in the coefficient matrix **k**.
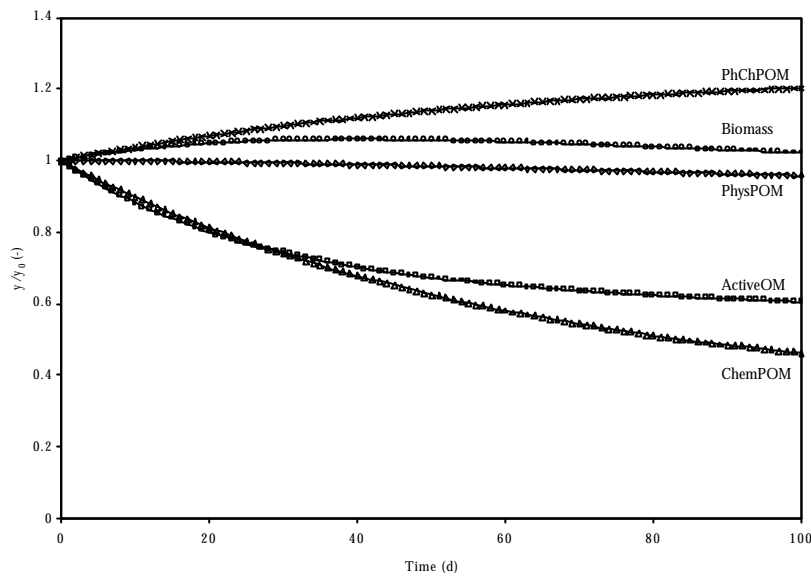
Figure 14-1. Comparison between analytical (lines) and numerical (symbols) relative changes of the five pools (y/y₀) as a function of time.

14.4 References

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15 User's guide

Marius Heinen

15.1 Model structure

Heinen and de Willigen (1998) described the structure of the model in their chapter 5 '*User's Guide*'. Of course, the main structure has not been changed much. To facilitate the understanding for the programmer, all integrating routines have been structured so that they consist of the following main structure elements (if applicable): initialize, rate, integrate (or state), output, terminal. These have been adopted from the FSE2 structure of van Kraalingen (1995). Such a structure consisting of rate and integrate sections is applicable for explicit integrations. For the implicit solution of the Richards equation this seems not applicable. The integrate section for the solution of the Richards equation is skipped when the time step has not been changed between the rate and integrate steps. If however, the time step Δt is changed (has become lower), the new status for water is computed as

```
state(t+Δt) = state(t) + rate(t+Δt)*Δt,
```

in which the rate of change was stored in the rate section

15.2 FUSSIM2 and FSE4

Since the previous version of FUSSIM2 (Heinen and de Willigen 1998) FUSSIM2 has been used extensively coupled with plant growth models. For this purpose FUSSIM2 and the crop growth models were coupled (not integrated) under FSE4 (Rappoldt, 2001). This means that the old MAIN of FUSSIM2 has been adapted so that it can be used as a subroutine that is called by FSE4. It goes beyond the scope of this report to describe the new features as they are directly related to the structure of FSE4, which is described in Rappoldt (2001). It suffices to mention here that it is possible to run FUSSIM2 stand-alone, i.e. not coupled to any other model. Coupling to dummy crop growth models (e.g. models that supply data from tables, such as LAI, nutrient demand, root growth rates) is also possible (e.g. de Vos en Heinen, 1999; Assinck and Heinen, 2001). Experience has shown, so far, that it is not easy to have a single, unique main FUSSIM2 subroutine that can handle all cases of running stand-alone or coupled to different types of crop growth models. Therefore, this subroutine, with the name FUSSIM2FSE4, is to be adapted for each specific project. With FSE4 reruns (van Kraalingen and Rappoldt, 2000) are still possible (see section 15.6).

In FUSSIM2 there is a main focus upon the interaction of soil processes and root uptake. Therefore, it is likely that pure stand-alone simulation of soil processes

hardly will occur. In other words, coupling to dummy or real plant growth models will occur most frequently. However, as a special option, we have integrated a expo-linear crop growth module and a nutrient demand module in FUSSIM2. These modules can be invoked by supplying some logicals and will be used each time step.

Evapotranspiration can be dealt with in several ways. The user can supply known potential transpiration T_p and potential evaporation E_p (ETMETH=0). Alternatively, FUSSIM2 can compute T_p and E_p according to three algorithms of van Kraalingen and Stol (1997) (ETMETH=1,2,3), or from user-supplied potential evpotranspiration rates ET_0 (ETMETH=4). For ETMETH > 0, additional information is required (see description of input file WEATHER in section 15.4.6).

15.3 Correspondence between variables in files and variables in text

Table 15-1 lists the input parameters required by the simulation model and the (possible) output variables. Table 15-2 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 15.5 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 error 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 (kg ha^{-1}).
- 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 (kg ha^{-1}).
- Total required uptake of solute(s) by the crop since $t = 0$ (kg ha^{-1})
- Total uptake of solute(s) by the crop since $t = 0$ (kg ha^{-1})
- Total amount of fertilizer application since $t = 0$ (kg ha^{-1})
- 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) (kg ha^{-1}).

- 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.

Table 15-1. Lists of input parameters required by the simulation model, and list of (possible) output variables which are given at user-supplied print times.

Input parameters

Water
  $N, M, ? x_I, ? z_J$
  For all (I,J): $?_r, ?_s, n, a_d, a_w, K_s, ?$
  Top boundary conditions
    Per $(I,1)$ type of condition
    Per time unit: rain/irrigation rate, E_p, T_p (only for root water uptake)
  Bottom boundary conditions
    Per (I,M) type of condition plus corresponding prescribed h or q
  $h_o(I,J)$
  $? t_i, ? t_{max}, ? t_{min}, t_f, ?, t_m$
  e_c, e_I, maximum number of iterations
  Initial $?_I, e_?$ (see Chapter 4)

Root water uptake
  $K_1, R_0, a, h_{r,1/2}$
  $L_{rv}(I,J)$ (if root growth give also k_L, t^* and start time, and $L_{rv,f}(I,J) = L_{rv}(I,J)$, see Chapter 7 of Heinen, 1997)

Solute transport
  $c_f, a_T, a_L, D_0, f_1(I,J), f_2(I,J), ?_I(I,J)$
  $c_0(I,J)$

Root nutrient uptake
  S_{sr}

Output variables (per printing time)

Water
  <optional> $?(I,J), h(I,J), q_x(i,j), q_z(i,j)$
    <always>   total water storage, total change in water storage since $t = 0$, water mass balance error, total amount of water that passed the boundaries

Root water uptake
  <optional> $S_w(I,J)$ (actual rate and cumulative since $t = 0$), h_r, T, total water uptake by plant roots

Nutrient transport
  <optional> $c(I,J), Q_m(I,J), EC(I,J), q_{sx}(i,j), q_{sz}(i,j)$,
    <always>   total nutrient storage, total change in nutrient storage since $t = 0$, solute mass balance error, total amount of nutrient that passed the boundaries

Root nutrient uptake
  <optional> $S_s(I,J)$ (actual rate and cumulative since $t = 0$), total nutrient uptake by plant roots

Table 15-2. 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 (references in italic refer to Heinen and de Willigen (1998), others to current report), 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 (alphabetically sorted) per input file, and only the most important variables are listed. Input files are described in more detail in Section 15.4.

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
INPUT.DAT (Section 15.4.1)					
AMMONIUMDAT	character*50				
BNAME	character*50				
EXPLINDAT	character*50				
EXTMAKEDAT	character*50				
FERTILDAT	character*50				
FLSALT	character*50				
FUS2CTR	character*50				
FUSSIM2LOG	character*50				
GWLDAT	character*50				
IONSINFODAT	character*50				
NITDENINDAT	character*50				
PHOSPHORDAT	character*50				
RNAME	character*50				
ROOTSDAT	character*50				
SLTNAM	character*50				
SNAME	character*50				
SOILSDB	character*50				
STEMPDAT	character*50				
TGENDAT	character*50				
THHFXFZDAT	character*50				
TNAME	character*50				
TRANSP	character*50				
TRANSPCTR	character*50				
UPTADAT	character*50				
VIMOKEDAT	character*50				
WETDAT	character*50				
WNAME	character*50				
FUS2.CTR (Section 15.4.2)					
ANSI	integer				
BIG	real		L		*[95], [96]*
DEPSAMNT	real				
DEPSLRV	real				
DEPSN	real				
DEPSP	real				
DEVDUM	real		the factor 100 in denominator of *Eqs. [133],[134]*	cm (*Eq. [133]*) or cm t^{-1} (*Eq. [134]*)	*[133], [134]*
DTFAC	real		m_t		*[181]*
DUMP	character*1				
FLSALT	character*1				
HSAT	real			cm	
IGRAV	integer				
IOFEX	integer				
IPRCT	integer				
IPRGRS	integer				
KHFACX	real				

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
KHFACZ	real				
LOGITS	integer				
METHIR	integer				
PLGROW	character*1				
PRTINY	real			t	
QALL	logical				
REDEV	logical				
SMALDT	real		? t_{min}	t	*3.5*
STSTAT	character*1				
TOODEV	real				
TRANSP	character*1				
UPTAKE	character*1				
WET	character*7				
WTYPE	character*9				
SOIL.DAT (Section 15.4.3)					
CTREAT	integer				
DX	real	1, NC	? x_I	cm	*[58]*
DZ	real	1, NL	? z_J	cm	*[59]*
FILNAM	character*40				
INSIDE	integer	1, NL, NL*NC			
IS	integer				
ISOIL	integer	1, NL, NL*NC			
KWAY	integer				
NC	integer		*N*		*3.2.2*
NL	integer		*M*		*3.2.2*
NSOILS	integer	= 5			
P	real		*p*	cm^{-1}	*[218,220]*
Q	real		*q*	cm^{-1}	*[218,220]*
SOILNS	character*20	NSOILS			
TITLE	character*72				
TRANSP	real		*T*	cm d^{-1}	*[219,220]*
BOUNDS.DAT (Section 15.4.4)					
DRRES	real			d^{-1}	*[15]*
FBOT	real	1, NC	q_G	cm d^{-1}	*[10]*
FBOTTOMBCT	real	= 100*NC	q_G	cm d^{-1}	*[10]*
FINTRN	integer	1, NL, NL*NC			
FLEFT	real	1, NL	q_G	cm d^{-1}	*[10]*
FLEFTBCT	real	= 100*NL	q_G	cm d^{-1}	*[10]*
FRIGHT	real	1, NL	q_G	cm d^{-1}	*[10]*
FRIGHTBCT	real	= 100*NL	q_G	cm d^{-1}	*[10]*
FTOPBCT	real	= 100*NC	q_G	cm d^{-1}	*[10]*
H0	real			cm	*[15]*
HBOT	real	1, NC	h_G	cm	*[9]*
HBOTTOMBCT	real	= 100*NC	h_G	cm	*[9]*
HINI	real	1, NL*NC	$h_{0,I,J}$	cm	*[17]*
HINTRN	integer	1, NL, NL*NC		cm	
HLEFT	real	1, NL	h_G	cm	*[9]*
HLEFTBCT	real	= 100*NL	h_G	cm	*[9]*
HRIGHT	real	1, NL	h_G	cm	*[9]*
HRIGHTBCT	real	= 100*NL	h_G	cm	*[9]*
HTOP	real	1, NC	h_G	cm	*[9]*
HTOPBCT	real	= 100*NC	h_G	cm	*[9]*
IBOT	integer	1, NC			
IBOTTOMBCT	integer	= 100*NC			

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
IDITCH?	integer	=20			
IINTRN	integer	1, NL, NL*NC			
ILEFT	integer	1, NL			
ILEFTBCT	integer	= 100*NL			
IRIGHT	integer	1, NL			
IRIGHTBCT	integer	= 100*NL			
ISEEP?	integer	= 20			
ITOP	integer	1, NC			
ITOPBCT	integer	= 100*NC		t	
JDITCH?	Integer	= 20			
JSEEP?	Integer	=20			
MAXPND	real		y_m	cm	6.2
NDITCH	integer				
NSEEP	integer				
ROUGH	real		n		(6-4)
TIMBOTTOMBC	real	= 100		t	
TIMLEFTBC	real	= 100		t	
TIMRIGHTBC	real	= 100		t	
TIMTOPBC	real	= 100		t	
TIMER.DAT (Section 15.4.5)					
CONDEL	integer				
CONPRI	integer				*3.5*
DELT	real		$? \, t_i$	t	*3.5*
DTMAX	real		$? \, t_{max}$	t	*[181]*
EPSIL	real		e_c		*3.3.3*
EPSILI	real		e_i		*3.3.2*
FUSOUT	logical				
HOUT	integer	= 10 (must be even)			
ICRIT	integer				
IHYST	integer				
ISOLVE	integer				
KAPPA	integer	1 or NL*NC	$?_h$		*4.2,[202]*
MAXIT	integer				
MAXITI	integer				
OUTYES	integer	4			
PRDEL	real			t	*3.5*
PRTIME	real	= 6000		t	*3.5*
SUBREG	integer	4			
TAU	real		$e_?$		*[201]*
TOL	real				
UNITS	character*1				
WCOUT	integer	= 10 (must be even)			
ZETA	real		$?$	cm^3 cm^{-3}	*[179]*
WEATHER.DAT (Section 15.4.6)					
COUNTR	character				
ECTRSH	real			dS m^{-1}	*5.3.2*
EPOT	real	= 527040	$q_G(t)$	cm t^{-1}	*[10]*
ET0	real	= 527040	$q_G(t) + T_p(t)$	cm t^{-1}	*[10]*
ETMETH	integer				
ETPTH	real			cm t^{-1}	*5.3.2*
FCROPS	real				

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
HTRESH	real			cm	*5.3.2*
IDOYFCR	integer				
IDOYLAI	integer				
IFCROP	integer				
IFLAG	integer				
IRRINT	real		q_G	$cm\,t^{-1}$	*[10],5.3.2*
ISTN	integer				
ISURF	integer				
ITRESH	integer				*5.3.2*
IYEAR	integer				
IYRFCR	integer				
IYRLAI	integer				
JTRESH	integer				*5.3.2*
KCROP	real				
LAIS	real				
LFRAC	real				*5.3.2*
LOGF	integer				
METHIR	integer				
PENMAN	character*2				
RAIN	real	= 527040	$q_G(t)$	$cm\,t^{-1}$	*[10]*
RF	real				
TDMI	real			^0C	
TPOT	real	= 527040	$T_p(t)$	$cm\,t^{-1}$	*[25]*
WTRDIR	character				
SOILS.DB (Section 15.4.7)					
TALP	real	= 100	a	cm^{-1}	*[182]*
TALPD	real	= 100	a_d	cm^{-1}	*[182]*
TALPW	real	= 100	a_w	cm^{-1}	*[182]*
TBNAME	character*20	= 100			
TKK	real	= 100	K_k	$cm\,d^{-1}$	(4-2)
TKS	real	= 100	K_S	$cm\,d^{-1}$	*[183,186]*
TL	real	= 100	$?$		*[183,186]*
TND	real	= 100	n		*[182]*
TNW	real	= 100	n_w		*[182]*
TWCR	real	= 100	$?_r$	$cm^3\,cm^{-3}$	*[182]*
TWCS	real	= 100	$?_s$	$cm^3\,cm^{-3}$	*[182]*
WCK	real	= 100	q_k	$cm^3\,cm^{-3}$	(4-7)
EXTMAKE.DAT (Section 15.4.8)					
ES0	real	= 50	E_p	$cm\,d^{-1}$	5.1
EXTMETHOD	character*8				
H	real	= 50	h_1	cm	5.1
METHOD	character*3				
MINT	character*4				
NNTAB	integer				
PPBIG	real			cm	
PPEND	real			cm	
PPREF	real			cm	
SCRNLOG	logical				
GWL.DAT (Section 15.4.9)					
DOYGWL	real	= 1000			
GWLS	real	= 1000		cm	

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
IYRGWL	integer	= 1000			
VIMOKE.DAT (Section 15.4.10)					
CDCORR	real		CF		(7-7)
HDRAIN	real	= 1000	h_{drain}	cm	7.2
IDOYDRAIN	integer	= 1000			
IDRAIN	integer	1			
IYEARDRAIN	integer	= 1000			
JDRAIN	integer	1			
NDRAIN	integer	1			
REFF	real		r	cm	(7-3)
THHFXFZ.DAT (Section 15.4.11)					
FX	real	NL*(NC+1)	q_x	mL cm^{-2} t^{-1}	*[1], [2]*
FZ	real	(NL+1)*NC	q_z	mL cm^{-2} t^{-1}	*[1], [2]*
H	real	NL*NC	h	cm	*[3]*
WC	real	NL*NC	$\boldsymbol{q}$	mL cm^{-3}	*[1], [2]*
WET.DAT (Section 15.4.12)					
XWET	real	= 50	h	cm	*[2], [182]*
YWET	real	= 50*NSOILS	$\boldsymbol{q}$	mL cm^{-3}	*[1], [182]*
STEMP.DAT (Section 15.4.13)					
CMETH	character*11				
DTSTEP	real		$? t$	d	(13-4)
METH1	character*7				
METHNL	character*7				
SOIL	character*4				
TC	real		t_c	d	(13-18)
TIMAV	real		t_{av}	d	(13-19)
TINI	real		t	d	(13-1), (13-19)
TYAMP	real		A_0	^{0}C	(13-16)
TYAV	real		T_{av}	^{0}C	(13-16)
SOLUTE.DAT (Section 15.4.14) below NION (= 13) represents the number of ions present in solution					
AL	real	1, NL, NL*NC	a_L	cm	*[33]*
AMOUNT	real	NION, NION*NL, NION*NL*NC	Q_m	mmol or mg	*[46]*
AT	real	1, NL, NL*NC	a_T	cm	*[33]*
BDS	real	1, NL, NL*NC		g cm^{-3}	
CBOT	real	NION, NION*NC	c_G	mmol	*2.5*
CF1	real	1, NL, NL*NC	f_1		*[34]*
CF2	real	1, NL, NL*NC	f_2		*[34]*
CLEFT	real	NION, NION*NL	c_G	mmol	*2.5*
CONC	real	NION, NION*NL, NION*NL*NC	C	mmol l^{-1}	*[45]*
CRIGHT	real	NION, NION*NL	c_G	mmol	*2.5*
CTOP	real	NION, NION*NC	c_G	mmol	*2.5*
FREQF	integer				
ICON	integer				
IDISP	integer				
JBOT	integer	1, NC			
JLEFT	integer	1, NL			
JRIGHT	integer	1, NL			
JTOP	integer	1, NC			
LD	real		L_D	cm	*[172]*
OUTSLT	integer	7			

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
WCLOW	real	1, NL, NL*NC	$?_l$	cm^3 cm^{-3}	*[34]*
AMMONIUM.DAT (Section 15.4.15) (parameters like for phosphorus)					
A1	real	1, NL, NL*NC	a_1	mg cm^{-3}	(8-10)
A2	real	1, NL, NL*NC	a_2	mg cm^{-3}	(8-10)
AK	real		a_k	mg cm^{-3} $(ml$ $mg^{-1})^{-1}$	8.5
B1	real	1, NL, NL*NC	b_1	ml mg^{-1}	(8-10)
B2	real	1, NL, NL*NC	b_2	ml mg^{-1}	(8-10)
FREUM	real		M	mg cm^{-3} $(ml$ $mg^{-1})^{-N}$	(8-11)
FREUN	real		N		(8-11)
LINPAR	logical				
MODPAR	logical				
OUTNH4	integer				
IONSINFO.DAT (Section 15.4.16)					
DEBYE	integer				
DIF0	real	13	D_0	cm^2 d^{-1}	*[33], [43]*
IONNAM	character*5	13			
IONRAD	real	13	d_i	Angstrom	*[37]*
IONYES	integer	13			
MOBIL	real	13	μ_m	cm s^{-1} V^{-1}	*[35], [43]*
PARA	real	13	A_f	$(mol$ $kg^{-1})^{0.5}$	*[38]*
PARAB	integer				
PARB	real	13	B_f	$(mol$ $kg^{-1})^{0.5}$ m^{-1}	*[39]*
VALENC	real	13	n_v		*[35], [36], [37], [43]*
NITDENIN.DAT (Section 15.4.17)					
NitSourceParam1	real		n_1	$mmol^2$ kg^{-2} (wet soil)	(12-1)
NitWaterParam1	real		n_2		(12-2)
NitWaterParam2	real		n_3		(12-2)
NitTempParam1	real		n_4		(12-3)
NitTempParam2	real		n_5		(12-3)
NitTempParam3	real		n_6		(12-3)
NitTempParam4	real		n_7		(12-3)
NitpHParam1	real		n_8		(12-4)
NitCECParam1	real		n_9	$mmol^2$ kg^{-2} (wet soil) d^{-1}	(12-5)
NitCECParam2	real		n_{10}	$mmol^2$ kg^{-2} (wet soil) d^{-1}	(12-5)
NitPartParam1	real		n_{11}		(12-6)
NitPartParam2	real		n_{12}		(12-6)
NitPartParam3	real		n_{13}		(12-6)
NitPartParam4	real		n_{14}		(12-6)
pHDepthTabel	real		pH		(12-4), (12-12)
CECDepthTabel	real		CEC	$cmol+$ kg^{-1}	(12-5)
DenSourceParam1	real		d_1	mol kg^{-1} (wet soil)	(12-7)
DenWaterParam1	real		d_2		(12-8)
DenWaterParam2	real		d_3		(12-8)
DenTempParam1	real		d_4		(12-9)
DenTempParam2	real		d_5		(12-9)
DenTempParam3	real		d_6		(12-9)
DenTempParam4	real		d_7		(12-9)
DenElectrParam1	real		d_8		(12-10), (12-11)
DenpHParam1	real		d_9		(12-12)

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
DenpHParam2	real		d_{10}		(12-12)
DenpHParam3	real		d_{11}		(12-12)
DenEmisParam1	real		e_2		(12-14)
DenEmisParam2	real		e_3		(12-14)
DenEmisParam3	real		e_4	d^{-1}	(12-14)
DenEmisParam4	real		e_1		(12-13)
N2OinAtmosphere	real		N_2O_{air}		(12-13)
GasConstant	real				
N2ODepthTabel	real				
N2DepthTabel	real				
DNPDepthTabel	real		DPR		(12-7)
PHOSPHOR.DAT (Section 15.4.18)					
A1	real	1, NL, NL*NC	a_1	mg cm^{-3}	(8-10)
A2	real	1, NL, NL*NC	a_2	mg cm^{-3}	(8-10)
AK	real		a_k	mg cm^{-3} (ml mg^{-1})$^{-1}$	8.5
ALFEOX	real	1, NL, NL*NC	[Al+Fe]	mmol kg^{-1}	(8-9)
ALPH1	real	1, NL, NL*NC	$\boldsymbol{a}_1$	d^{-1}	(8-8)
ALPH2	real	1, NL, NL*NC	$\boldsymbol{a}_2$	d^{-1}	(8-8)
ALPH3	real	1, NL, NL*NC	$\boldsymbol{a}_3$	d^{-1}	(8-8)
B1	real	1, NL, NL*NC	b_1	ml mg^{-1}	(8-10)
B2	real	1, NL, NL*NC	b_2	ml mg^{-1}	(8-10)
BI1	real	1, NL, NL*NC	b_1	(mg L^{-1})$^{-N1}$	(8-9)
BI2	real	1, NL, NL*NC	b_2	(mg L^{-1})$^{-N2}$	(8-9)
BI3	real	1, NL, NL*NC	b_3	(mg L^{-1})$^{-N3}$	(8-9)
FREUM	real		M	mg cm^{-3} (ml mg^{-1})$^{-N}$	(8-11)
FREUN	real		N		(8-11)
LINPAR	logical				
MODPAR	logical				
N1	real	1, NL, NL*NC	N_1		(8-8)
N2	real	1, NL, NL*NC	N_2		(8-8)
N3	real	1, NL, NL*NC	N_3		(8-8)
OUTADS	integer	4			
PW	real	1, NL, NL*NC	P_w	mg P$_2$O$_5$ L^{-1} (soil)	(8-16)
REDF	real	1, NL, NL*NC			
UPTA.DAT (Section 15.4.19)					
CMIN	real	13	C_{min}	mg mL^{-1}	(9-4)
FMAX	real	13		mmol cm^{-2} d^{-1}	*3.4.3*
IUPMAX	integer				
IUPWAY	integer				
METHODU	integer				
UPCRIT	real				
TRANSP.DAT (Section 15.4.20)					
A	real	NPLANT	a		*[26]*
HOSP	real	NPLANT	$h_{o,r}$	cm	*[20]*
HRHALF	real	NPLANT	$h_{r,1/2}$	cm	*[26]*
K1	real	NPLANT	K_1	cm d^{-1}	*[20]*
LRVINI	real	NL*NC	L_{rv} ($t = 0$)	cm cm^{-3}	*[19]*
LRVK	real	NPLANT	$LRVK$	d^{-1}	*[203]*
LRVT	real	NPLANT	$LRVT$	d	*[203]*
LRVTS	real	NPLANT	$LRVTS$	d	*[203]*
OUTTRA	integer	6			
R0	real	NPLANT	R_0	cm	*[21]*

Variable names in input files	Type of variable	Number of array entries	Variables used in text	Dimension	Equation Section
REDPOT	integer				
RTGROW	integer				
SIGMA	real	NPLANT	s_r		*[20]*
TRANSP.CTR (Section 15.4.21)					
FAC	real				*3.2.5*
NP	integer				
RDPMIN	real		e_t		*[112]*
TOL	real				
TRANS	character*7				
TRHYST	character*1				
TGEN.DAT (Section 15.4.22)					
NNTAB	integer				
PPBIG	real			cm	
PPEND	real			cm	
PPREF	real			cm	
EXPLIN.DAT (Section 15.4.23)					
A	real	NPLANT*NION	a_G	g g^{-1}	(10-6)
B	real	NPLANT*NION	b_G	g g^{-1}	(10-6)
C	real	NPLANT*NION	c_G	ha kg^{-1}	(10-6)
CM	real	NPLANT	c_m	kg ha^{-1} d^{-1}	(10-1)
DEMMOD	logical				
DM	real	NDM = 10	W_T	kg ha^{-1}	10.3 (tabulated data)
FMAX	real	NPLANT*NION		mmol cm^{-2} d^{-1}	*3.4.3*
NPLANT	integer	= 5			
OPTC	real	NDM*NPLANT*NION	N_O	g g^{-1}	10.3 (tabulated data)
PL	real	NPLANT	P_L	g g^{-1}	(10-5)
PLNUM	integer	1, NC			
RM	real	NPLANT	r_m	kg ha^{-1} d^{-1}	(10-1)
SHRT	real	NPLANT	*SHRT*	g g^{-1}	(10-4)
SLA	real	NPLANT	*SLA*	ha kg^{-1}	(10-5)
TCNU	real	NPLANT*NION	t_N	d	(10-11)
TUPT	real	NPLANT*NION	U	kg ha^{-1}	(10-7)
WTOT	real	NPLANT	W_T	kg ha^{-1}	(10-1)
ROOTS.DAT (Section 15.4.24)					
DECRAT	real	NPLANT	l_L	d^{-1}	(11-1)
DMCR	real	NPLANT	DM_r	g g^{-1}	(11-4)
LRVINI	real	NPLANT*NL*NC	L_{rv}	cm cm^{-3}	(11-1)
QIN	integer	NPLANT*NL*NC	related to Q_L		(11-1), (11-4)
R0	real	NPLANT	R_0	cm	(11-4)
RDX0	real	NPLANT	D_{Lx}	cm^2 d^{-1}	(11-1)
RDZ0	real	NPLANT	D_{Lz}	cm^2 d^{-1}	(11-1)
REDH	real	12			
RHOR	real	NPLANT	r_r	g cm^{-3}	(11-4)
FERTIL.DAT (Section 15.4.25)					
FCOL	integer	= 50			
FERTTM	real	= 10		d	
FFERT	real	= 10*MAXION		kg ha^{-1}	
FROW	integer	= 50			

15.4 Description of input files

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 Van Kraalingen and Rappoldt (2000). The rules are:

- array elements should be separated by a space or a comma;
- arrays may also be given in column format with array name on separate line; e.g.
  ```
  AR1  AR2  AR3
  1.0  1.4  2.0
  3.3  0.5  1.1
  ```
- 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 between single quotes;
- integer values must be given as integers;
- real values must be given as reals;
- if an array consists of only 1 element it must be given as 1*value, e.g. A = 1*2.5 and not A = 2.5
- position of variable name in data file is free;
- extra variable names may be present;
- information behind a "*" (first column) or a "!" (any column) 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. Table 15-3 gives the maximum values or number of array elements for some of the variables.

In the example input files described in the following sub-sections, all required and optional variables are presented. Required variables are presented first, while optional variables are listed at the bottom of the example input files. Optional variables are printed in italic, and the values given to these optional variables are the values used by FUSSIM2 as default values when the optional variable is not present in the input file. Generally, these optional variables should be used only by experienced users.

Table 15-3. Maximum value or maximum number of array elements for several variables.

Variable	Maximum value	Maximum number of elements
EPOT, ET0, RAIN, TPOT		527040
IDITCH?, JDITCH?		100*NDITCH
ISEEP?, JSEEP?		100*NSEEP
NC, NL	100	
NDITCH	5	
NION	13	
NPLANT	5	
NSEEP	5	
NSOILS	10	
PRTIME		6000
XWET, YWET		50, 50*NSOILS
TBNAME, TKK, TKS, TWCS, TWCR , TWCK, TND, TNW, TALP, TALPD TALPW, TL		100

15.4.1 Input file INPUT.DAT

FUSSIM2 reads data from input files. Some names for data files are required, in other cases names are optional or have default names if not given by the user. The user must supply the relevant names for data files in the special data file INPUT.DAT (name cannot be changed). Table 15-4 summarizes all possible data files that a user can supply, indicating which are required, which are optional and which have default names if not supplied. Also indicated are the modules of FUSSIM2 that uses the data file. Although 28 files have been listed in Table 15-4, the user is free to combine data in only a few files by giving several of the variables the same file name. For example, if the user wants to put all variables necessary for transpiration into one file named MYTRANS.DAT, then in the file INPUT.DAT the following lines must be given:

```
TRANSP       = 'MYTRANS.DAT'
TRANSPCTR    = 'MYTRANS.DAT'
TGENDAT      = 'MYTRANS.DAT'
```

Table 15-4. Explanation of all possible files names that must or can be supplied in the file INPUT.DAT.

```
Explanation of column required:
   R  = required: name must be supplied
   RO = required, but name is optional (else default name is used)
   O  = file only necessary in certain cases, name is optional (else default
        name is used)


Explanation of the abbreviation of the modules
   wa = water, sl = solute, te = temperature, tr = transpiration, up = uptake

#   name                 required    default name            modules
                         (R,RO,O)                            wa  sl  te  tr  up
-----------------------------------------------------------------------------
 1  FUS2CTR              RO      FUS2.CTR
 2  FUSSIM2LOG           RO      FUSSIM2.LOG
 3  SOIL    or SNAME     R                                    +
 4  BOUNDS  or BNAME     R                                    +
 5  TIMER   or TNAME     R                                    +
 6  WEATHER or WNAME     R                                    +
```

```
 7   SOILSDB              O    as supplied in SNAME   +
 8   RNAME          R                                 +
 9   EXTMAKEDAT         RO     EXTMAKE.DAT            +
10   GWLDAT               O    GWL.DAT               +
11   VIMOKEDAT          RO     VIMOKE.DAT            +
12   THHFXFZDAT           O    THHFXFZ.DAT           +
13   WETDAT               O    WET.DAT               +
14   STEMPDAT           RO     STEMP.DAT                      +
15   SOLUTE or FLSALT  R                                 +
16   SLTNAM         R                                 +
17   AMMONIUMDAT          O    AMMONIUM.DAT          +
18   IONSINFODAT        RO     IONSINFO.DAT          +
19   NITDENINDAT          O    NITDENIN.DAT          +
20   PHOSPHORDAT          O    PHOSPHOR.DAT          +
21   UPTADAT            RO     UPTA.DAT                          +
22   TRANSP         R                                      +
23   TRANSPCTR          RO     TRANSP.CTR                 +
24   TGENDAT            RO     TGEN.DAT                   +
25   EXPLINDAT          RO     EXPLIN.DAT            for experienced users only
26   ROOTSDAT           RO     ROOTS.DAT
27   FERTILDAT            O    FERTIL.DAT            +

 #   name           description
-----------------------------------------------------------------------
 1   FUS2CTR        some control data for FUSSIM2
 2   FUSSIM2LOG     log file for FUSSIM2
 3   SOIL/SNAME     definition of soil domain, CVs, soil types
 4   BOUNDS/BNAME   initial and boundary conditions for water movement
 5   TIMER/TNAME    timer and control data for water movement
 6   WEATHER/WNAME  some atmospheric data
 7   SOILSDB        name of soils data base file [overruling name supplied in SOIL]
 8   RNAME          name of output file for water movement
 9   EXTMAKEDAT     data file for making soil evaporation reduction table
10   GWLDAT         groundwater levels as specific bottom boundary condition
11   VIMOKEDAT      Vimoke drain data file
12   THHFXFZDAT     steady-state water movement: status distribution
13   WETDAT         tabulated wetting curve
14   STEMPDAT       soil temperature data file
15   SOLUTE/FLSALT  initial and boundary conditions for solute transport
16   SLTNAM         name of output file for solute transport
17   AMMONIUMDAT    data file if ammonium adsorption is to be considered only if NH4
                    is indicated in IONSINFODAT if AMMONIUMDAT = 'NONE' or 'none'
                    then NO ammonium adsorption is considered
18   IONSINFODAT    which ions are to be considered and some of their properties
19   NITDENINDAT    data file for nitrification and denitrification module only if
                    NO3 and NH4 are indicated in IONSINFODAT if NITDENINDAT = 'NONE'
                    or 'none' then NO nitrification and denitrification is considered
20   PHOSPHORDAT    data file if phosphorus adsorption is to be considered only if P
                    is indicated in IONSINFODAT if PHOSPHORDAT = 'NONE' or 'none'
                    then NO phosphorus adsorption is considered
21   UPTADAT        data file for nutrient uptake
22   TRANSP         data file for water uptake or transpiration
23   TRANSPCTR      control file for water uptake or transpiration
24   TGENDAT        control file for water uptake or transpiration
25   EXPLINDAT      data file for expo-linear growth module
26   ROOTSDAT       data file for root growth by diffusion
27   FERTILDAT      times of fertilization
```

Table 15-5 gives an example of the data file INPUT.DAT. Note that a path-structure can be given as well.

Table 15-5. Example input file INPUT.DAT.

```
! required names
SOIL    = 'input\heino_so'
BOUNDS  = 'input\heino_bc'
TIMER   = 'input\heino_tm'
WEATHER = 'input\heino_wh'
TRANSP  = 'input\heino_tr'
SOLUTE  = 'input\heino_sl'

RNAME   = 'output\heino_w'
SLTNAM  = 'output\heino_s'

! optional names
FUS2CTR      = 'input\fus2.ctr'
FUSSIM2LOG   = 'output\fussim2.log'
EXTMAKEDAT   = 'input\extmake.dat'
STEMPDAT     = 'input\stemp.dat'
AMMONIUMDAT  = 'NONE'
IONSINFODAT  = 'input\ionsinfo.dat'
NITDENINDAT  = 'input\nitdenin.dat'
PHOSPHORDAT  = 'NONE'
UPTADAT      = 'input\upta.dat'
TRANSPCTR    = 'input\transp.ctr'
TGENDAT      = 'input\tgen.dat'
```

In sections 15.4.2 until 15.4.25 the input files are described.

15.4.2 Input file FUS2.CTR

The file FUS2.CTR (example in Table 15-6) 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 (see section 15.4.11) 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.

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:

IRRINT   irrigation intensity (cm per time units)

ETPTH   threshold evapotranspiration (cm)

LFRAC   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))

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:

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)*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)*ETPTH (see above)

ECTRSH   threshold value of electrical conductivity (dS m-1)

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 a_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 (see section 15.4.12).

Table 15-6. Example input file FUS2.CTR. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
******* which processes to consider
TRANSP = 'N'                ! Yes or No include TRANSP
FLSALT = 'Y'                ! Yes or No include FLSALT
UPTAKE = 'N'                ! Yes or No include NUTUPT
PLGROW = 'N'                ! Yes or No include PLANT


******* data read by unit INIT
* Type of weather data input
*    WTYPE = 'FUSSIMOWN': according to FUSSIM format
*    WTYPE = 'SHELL"    : weather supplied by FSE4 shell
WTYPE = 'FUSSIMOWN'

* How to treat the wetting curve
*    WET = GENUCHT : use Van Genuchten parameters (default)
*    WET = LINEAR  : use linear interpolation
*    WET = SPLINE  : use cubic spline interpolation
WET = 'GENUCHT'

* Yes or No consider steady state condition.
STSTAT = 'N'

* Method of irrigation control
*    METHIR = 0 : times of irrigation given as input (default)
*    METHIR = 1 : irrigation when sum ETpot exceeds threshold
*    METHIR = 2 : irrigation when h exceeds threshold
*    METHIR = 3 : irrigation when EC exceeds threshold
METHIR = 0

* Type of logging of progress in time
*    IPRGRS = -1: no screen logging
*    IPRGRS =  0: log current time
*    IPRGRS =  1: log percentage time
IPRGRS = 0

* Print each IPRCT when IPGRS = 1
IPRCT = 5

* Yes (1) or not (0) log time and number of iterations to log file
LOGITS = 1

******* data read by unit CHDELT
* Increasing factor for time step (CONDEL <> 1) if negative, time step will
not be
```

```
* increased
DTFAC = 1.5D0


* Yes (TRUE) or not (FALSE) consider expo-linear growth
ELGROW = .FALSE.



* Yes (TRUE) or not (FALSE) consider nutrient demand module
NUTDEM = .FALSE.


* Yes (TRUE) or not (FALSE) consider root growth described as a diffusion
process
RGROW = .FALSE.


* Yes (TRUE) or not (FALSE) compute evaporation reduction at soil surface
REDEV = .TRUE.


******* data read by unit SOLVE
* The factor in the denominator of Eqs. [133] or [134]
* preferably 100; alternative may be 0
DEVDUM = 100.0D0


* If convergence criterion exceeds TOODEV then time step reduction occurs
TOODEV = 50.0D0


* No longer used
HSAT = -1.0D0


* Smallest allowable time step before program halts
SMALDT = 1.0D-15



* Large number used to handle Dirichlet boundaries
BIG = 1.0D25


******* for time step regulation
DEPSN    = 0.1            ! maximum allowable relative change of N processes
                         !    (ammonium    adsorption,    nitrification-
denitrification)
DEPSP    = 0.1           ! maximum allowable relative change of P processes
DEPSLRV  = 0.1           ! maximum allowable relative change of Lrv
DEPSWTOT = 0.1           ! maximum allowable relative change of WTOT
(EXPLIN)
DEPSAMNT = 0.1           ! maximum allowable relative change of total
amount of a
                         ! nutrient


******* data read by unit KAVER
* increase factor for horizontal conductivity with respect to vertical
* conductivity; to simulate anisotropy
KHFACX = 1.D0
* increase factor for vertical conductivity with respect to horizontal
* conductivity; to simulate anisotropy
KHFACZ = 1.D0


******* data read by unit WROUT
DUMP   = 'N'             ! Yes or No use ASCII dump as output (do not
change)
PRTINY = 1.0D-10         ! print control; do not change
QALL   = .TRUE.          ! print cumulative flow across boundaries for each
type
                         ! of boundary condition plus net totals
```

```
* Yes (1) or not (0) the DOS screen can handle ANSI escape sequence
controls.
ANSI = 0

* Yes (1) or no (0) do inquire on existence of output file.
IOFEX = 0

* Yes (1) or not (0) include gravity
IGRAV = 1

* Yes or No consider irrigation at bottom (for experienced users only).
BOTIRR = 'N'
```

15.4.3 Input file SOIL.DAT

In this input file general information about the flow domain is given (example in
Table 15-7), 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 of Heinen and de Willigen (1998).

FILNAM
The file FILNAM contains the Van Genuchten-Mualem parameters in tabulated
form for the given soil name SOILNS (see section 15.4.7). This name can be
overruled by the name SOILSDB as supplied in INPUT.DAT.

NSOILS, SOILNS, ISOIL
The number of different soil types is NSOILS. These types are given a name
(SOILNS) which appears in FILNAM. All control volumes should obtain a code
ISOIL (from 1 through NSOILS) linking them to the hydraulic properties of the
corresponding soil.

CTREAT   <optional>
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 of Heinen and de Willigen, 1998), or treated as a
constant (CTREAT = 2; used in example 6.1 of Heinen and de Willigen, 1998). In
case CTREAT = 1, the a parameter in the exponential expression becomes equal to
the a given in the Van Genuchten table. In case CTREAT = 2 the constant hydraulic
conductivity (CONCON) and constant differential moisture capacity should be
supplied (CONCAP).

IS   <optional>

With the variable IS = 1 (see example 6.2 of Heinen and de Willigen, 1998), 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.

TRANSP	transpiration rate (cm d^{-1})
P	extinction coefficient in *x* direction (cm^{-1})
Q	extinction coefficient in *z* direction (cm^{-1})

Table 15-7. Example input file SOIL.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* 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 (max. 72 characters)
TITLE = 'Test run, zandb1'

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

* Inside codes
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
INSIDE = 1*1

* thickness of soil columns DX (1 or NC values) and thickness of soil layers DZ
* supply 1 (all columns (DX) or rows (DZ) the same value), or NC (columns) or NL
* (rows) values
DX = 10*10.0
DZ = 16*5.0, 10*2.0

* soil physical properties of the soil
* NSOILS : number of different soil types
* FILNAM : (path +)name of database file where properties are stored
* SOILNS : 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.DB'
SOILNS = 1*'zandb1'

* give soil code to each control volume:
* supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
ISOIL = 1*1

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

```
CTREAT = 0

* 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; default)
* If IS = 1 then supply values for P(1/cm), Q(1/cm) and TRANSP (cm/d) especially
* for example 6.2 of Heinen and de Willigen (1998)
IS = 0
```

15.4.4 Input file BOUNDS.DAT

This file contains the (time independent) boundary conditions, internal conditions, and initial *h* distribution (example in Table 15-8). Time variable boundary conditions, in this case rain or irrigation and evapotranspiration data, are given in the file WNAME.

HINI
The initial pressure head distribution is supplied as HINI. For all control volumes a pressure head should be supply (NL*NC values). If the initial pressure head distribution is that of an equilibrium situation the user can supply one single value for HINI (HINI = 1*value) which represents the pressure head of the bottom layer. The program automatically computes the pressure head distribution of all other nodes. The volumetric water content and hydraulic conductivity are computed from the initial pressure head distribution based on value of KAPPA (in TIMER.DAT).

NSEEP, ISEEP, JSEEP   <optional>
The variable NSEEP contains the number of seepage faces present in the flow domain (= 5). For each of the seepage faces the column (ISEEP?) and row (JSEEP?) 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: NSEEP = 2, and data for the arrays ISEEP1, JSEEP1, and ISEEP2, JSEEP2. Note that when considering a seepage face at the bottom you must indicate for these nodes IBOT = 0.

NDITCH, IDITCH, JDITCH<optional>
For special cases the net outflow through ditch walls can be obtained by indicating which nodes (IDITCH?, JDITCH?; see description above for NSEEP, ISEEP, JSEEP) are involved. This results in extra output variable in the water output file RNAME.

Table 15-8. Example input file BOUNDS.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* data file for program FUSSIM2 containing boundary, internal and initial
* conditions for water

* boundary conditions can either be constant or time-dependent; for constant
* boundary conditions the following variables should be supplied (if applicable):
* ITOP, HTOP, IBOT, HBOT, FBOT, ILEFT, HLEFT, FLEFT, IRIGHT, HRIGHT, FRIGHT
* for time-dependent boundary conditions the following variables should be supplied
* (if applicable):
* TIMETOPBC,    ITOPBCT,    HTOPBCT
* TIMEBOTTOMBC, IBOTTOMBCT, HBOTTOMBCT, FBOTTOMBCT
* TIMELEFTBC,   ILEFTBCT,   HLEFTBCT,   FLEFTBCT
* TIMERIGHTBCT, IRIGHTBCT,  HRIGHTBCT,  FRIGHTBCT
* Below only examples for constant boundary conditions are given. For time-
* dependent conditions the times should be given with corresponding conditions
* which can have the values as those for the constant conditions. For example:
* TIMELEFTBC =    0.0      365.0      366.0    730.0
* ILEFTBCT   = 26*0       26*0       26*-1     26*-1
* HLEFTBCT   = 26*0.0     26*0.0     26*10.0   26*10.0
* FLEFTBCT   = 26*0.0     26*0.0     26*0.0    26*0.0
* Which indicates that between for the time-interval [0,365] ILEFT = 0 (HLEFT and
* FLEFT have no meaning in that case), and that for the time-interval [366-730] a
* fixed pressure head HLEFT = 10.0 is required (FLEFT has no meaning).
* Note that linear interpolation between times is done. Especially for changing
* boundary types (e.g. ILEFT) this may cause problems.
* Note that for each time NC (for top and bottom) or NL (for left or right) values
* for IxxxBCT, HxxxBCT and FxxxBCT must be supplied.
* Time dependent boundary conditions are used when TIMExxxBC is present. If not
* present, the constant boundary conditions are used.

* ITOP: pointer to boundary condition at top
*   ITOP < 0 : prescribed pressure head (HTOP) at top boundary
*   ITOP = 0 : no flux across top boundary
*   ITOP = 1 : flux equal to input by rain and/or irrigation only
*   ITOP = 2 : flux equal to output due to evaporation only
*   ITOP = 3 : flux equal to difference in input and output (default)
* Supply either 1 (all columns the same condition) or NC values for ITOP
* For HTOP you must supply exactly the same amount of values as for ITOP
ITOP   = 10*3


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

* IBOT: pointer to boundary condition at bottom
*   IBOT = -4 : time-dependent groundwater levels as specified in GWL.DAT (must be
*               supplied for all columns)
*   IBOT <  0 : prescribed pressure head (HBOT) at lower boundary (except when
*               IBOT = -4)
*   IBOT =  0 : seepage drainage at lower boundary
*               NB: you must also supply variable NSEEP 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)
* Supply either 1 (all columns the same condition) or NC values for IBOT
* For HBOT, FBOT you must supply exactly the same amount of values as for IBOT
IBOT   = 10*1

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

```
* known flux at bottom; only of importance if IBOT = 1 (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
* Supply either 1 (all rows the same condition) or NL values for ILEFT
* For HLEFT, FLEFT you must supply exactly the same amount of values as for ILEFT
ILEFT  = 25*1,-1

* constant pressure head at bottom; only of importance if ILEFT < 0
HLEFT  = 26*0.0

* known flux at bottom; only of importance if ILEFT = 1 (cm/d)
* program converts units corresponding to UNITS as supplied in timer file
FLEFT  = 26*0.0

* right boundary conditions
* IRIGHT: pointer to boundary condition at right boundary
*    IRIGHT < 0 : prescribed pressure head (HRIGHT) at right boundary
*    IRIGHT = 0 : no flow at right boundary
*    IRIGHT > 0 : prescribed flux (FRIGHT) at right boundary
* Supply either 1 (all rows the same condition) or NL values for IRIGHT
* For HRIGHT, FRIGHT you must supply exactly the same amount of values as for
* IRIGHT
IRIGHT = 10*1, 16*-1

* constant pressure head at bottom; only of importance if IRIGHT < 0
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.

* known flux at bottom; only of importance if IRIGHT = 1 (cm/d)
* program converts units corresponding to UNITS as supplied in timer file
FRIGHT = 26*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
* Supply 1 (equilibrium condition with HINI for all nodes at the bottom), or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
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  -42.5
     -87.5  -80.0  -75.0  -70.0  -65.0  -60.0  -55.0  -50.0  -45.0  -37.5
     -82.5  -75.0  -70.0  -65.0  -60.0  -55.0  -50.0  -45.0  -40.0  -32.5
     -77.5  -70.0  -65.0  -60.0  -55.0  -50.0  -45.0  -40.0  -35.0  -27.5
     -72.5  -65.0  -60.0  -55.0  -50.0  -45.0  -40.0  -35.0  -30.0  -22.5
     -67.5  -60.0  -55.0  -50.0  -45.0  -40.0  -35.0  -30.0  -25.0  -17.5
     -62.5  -55.0  -50.0  -45.0  -40.0  -35.0  -30.0  -25.0  -20.0  -12.5
     -57.5  -50.0  -45.0  -40.0  -35.0  -30.0  -25.0  -20.0  -15.0   -7.5
     -52.5  -45.0  -40.0  -35.0  -30.0  -25.0  -20.0  -15.0  -10.0   -2.5
     -47.5  -40.0  -35.0  -30.0  -25.0  -20.0  -15.0  -10.0   -5.0    2.5
     -42.5  -35.0  -30.0  -25.0  -20.0  -15.0  -10.0   -5.0    0.0    7.5
     -37.5  -30.0  -25.0  -20.0  -15.0  -10.0   -5.0    0.0    5.0   12.5
     -32.5  -25.0  -20.0  -15.0  -10.0   -5.0    0.0    5.0   10.0   17.5
     -27.5  -20.0  -15.0  -10.0   -5.0    0.0    5.0   10.0   15.0   22.5
     -22.5  -15.0  -10.0   -5.0    0.0    5.0   10.0   15.0   20.0   27.5
```

```
    -19.0   -11.5    -6.5    -1.5     3.5     8.5    13.5    18.5    23.5    31.0
    -17.0    -9.5    -4.5     0.5     5.5    10.5    15.5    20.5    25.5    33.0
    -15.0    -7.5    -2.5     2.5     7.5    12.5    17.5    22.5    27.5    35.0
    -13.0    -5.5    -0.5     4.5     9.5    14.5    19.5    24.5    29.5    37.0
    -11.0    -3.5     1.5     6.5    11.5    16.5    21.5    26.5    31.5    39.0
     -9.0    -1.5     3.5     8.5    13.5    18.5    23.5    28.5    33.5    41.0
     -7.0     0.5     5.5    10.5    15.5    20.5    25.5    30.5    35.5    43.0
     -5.0     2.5     7.5    12.5    17.5    22.5    27.5    32.5    37.5    45.0
     -3.0     4.5     9.5    14.5    19.5    24.5    29.5    34.5    39.5    47.0
      0.0     7.5    12.5    17.5    22.5    27.5    32.5    37.5    42.5    50.0

* number of seepage faces
NSEEP  = 1
* for seepage face 1 column (ISEEP1) and row (JSEEP1) numbers are given
ISEEP1 = 20*1
JSEEP1 =  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21,
         22, 23, 24, 25

* the pressure head of the seepage face during seepage; if not present the default
* value of zero is used
HSEEP = 0.0

* number of ditch walls
* if NDITCH > 0 then supply also IDITCH? and JDITCH? in a similar way as for
* seepage faces
NDITCH = 0

* internal conditions (NOT FULLY TESTED)
* IINTRN: pointer to boundary condition at internal node
*   INTRN < 0 : prescribed pressure head (HINTRN) at internal node
*   INTRN > 0 : prescribed flux (FINTRN) at internal node
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
IINTRN = 1*0
HINTRN = 1*0.0
FINTRN = 1*0.0
```

15.4.5 Input file TIMER.DAT

Data file containing general variables controlling computations of FUSSIM2 (example in Table 15-9). 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 requires 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.

$\quad\quad$ ISOLVE = 0 $\quad$ ICCG method (default)

$\quad\quad$ ISOLVE = 9 $\quad$ alternative, mostly faster solution procedure taken from the IMSL library; this solution procedure has been invoked at the time this report was written and has not been fully tested; if problems arise please use ISOLVE = 0

$\quad\quad$ ISOLVE = -1 solution procedure for one-dimensional situations (e.g. when NC = 1, or when no water flow may occur between columns)

In the previous version of FUSSIM2 (Heinen and de Willigen, 1998) the ADI method was described. Since then the ADI method has not been maintained. We do not take any responsibilities when the user supplies a value for ISOLVE in the range 1 through 4.

$\quad\quad$ ISOLVE = 1 $\quad$ ADI method, use Eqs. [116]-[121] of Heinen and de Willigen (1998) when unsaturated, use Eqs. [122]-[127] of Heinen and de Willigen (1998) when (partly) saturated; change between the two methods at pressure head HSAT as defined in file FUS2.CTR

$\quad\quad$ ISOLVE = 2 $\quad$ ADI method, use Eqs. [116]-[121] of Heinen and de Willigen (1998) all the times (when partly saturated conditions occur, the program generally crashes)

$\quad\quad$ ISOLVE = 3 $\quad$ ADI method, use Eqs. [122]-[127] of Heinen and de Willigen (1998) (large mass balance errors can be expected)

$\quad\quad$ ISOLVE = 4 $\quad$ 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 15-9. Example input file TIMER.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Data file for program FUSSIM2 containing time control data and iterations
* stop criterion

* Time units, must be in set [d, h, min, s]
* NOTE that all input variables in which time appears in the units should be given
* with time as days; the program converts units corresponding to UNITS as supplied
* in timer file. This counts for:
*    KS, KK, FBOT, FLEFT, FRIGHT, FINTRN, CONCON, TRANSP, DRRES
*    K1, LRVK, LRVT, LRVTS                    (module TRANSP)
*    FMAX, PLUPT, DIF0                        (module SOLUTE)
*    RDX0, RDZ0, DECRAT, RM, CM, TCNU, FMAX    (module PLANT)
* NOTE that : RAIN, TPOT, EPOT and IRRINT must be given with time equal to UNITS!
UNITS  = 'd'

* Initial time step in UNITS
DELT = 1.0E-5

* Maximum allowable time step in UNITS
DTMAX = 2.5E-1

* Is FUSSIM2 output needed (TRUE) or not (FALSE)
FUSOUT = .TRUE.

* If FUSOUT = .TRUE. then supply CONDEL, CONPRI, PRDEL, PRTIME
* CONDEL is optional; the default value when not present in this file: CONDEL = 0

* Maximum allowable change in water content used to determine new time step (if
* CONDEL = 0)
ZETA = 0.01

* Use constant print interval (CONPRI = 1) or not (CONPRI = 0)
CONPRI = 1

* Constant print interval (if CONPRI = 1) in UNITS
PRDEL = 1.0

* Times when to print results (if CONPRI = 0) in UNITS; must be in ascending order
PRTIME = 0.0 10.0 15.0 16.0 20. 300.

* Iterations stop criterion, e.g. 1.0E-4
EPSIL = 1.0E-04

* Maximum number of iterations due to non-linearity
MAXIT = 20

* Iterations stop criterion for ICCG0 method (ISOLVE = 0), e.g. 1.0E-8
EPSILI = 1.0E-08

* Maximum number of iterations for ICCG0 method (ISOLVE = 0)
MAXITI = 2000

* Is hysteresis to be considered
*   IHYST = 0: do not consider hysteresis
*   IHYST = 1: do consider hysteresis
IHYST = 0

* Initial hysteresis status for all nodes (KAPPA)
*    KAPPA = -2: start on main drying curve
*    KAPPA = -1: start on scanning drying curve
```

```
*     KAPPA = +1: start on scanning wetting curve
*     KAPPA = +2: start on main wetting curve
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
KAPPA = 1*-2

* What output is desired
OUTYES = 0,          ! print water content results: 1: yes, 0: no
         1,          ! print pressure head results: idem
         1,          ! print fluxes in x direction results: idem
         1           ! print fluxes in z direction results: idem

* Use constant time step (CONDEL = 1) or not (CONDEL = 0)
CONDEL = 0

* Type of convergence check
*   ICRIT =  0: use H and HLAST for DEVMAX
*   ICRIT =  1: use CON and KLAST for DEVMAX
*   ICRIT = -1: use cases 0 and 1 together (default when ICRIT is not present)
ICRIT = -1

* What solution procedure to use
*   ISOLVE = 0: use ICCG solution procedure (default)
*   ISOLVE = 9: use alternative IMSL solution method (not yet fully tested)
* Note that old ISOLVE options 1, 2, 3, and 4 (see Heinen and de Willigen, 1998)
* are no longer advised, i.e. these methods have not been maintained since 1998.
ISOLVE = 0

* If IHYST = 1 then supply TAU and TOL
*   TAU: control variable for change of status determination, e.g. 0.01
*   TOL: convergence criterion for zero-point determination in ZBRENT
TAU = 1.0E-2
TOL = 1.0E-6

* Sub-region for which totals are to be printed.
* Must consist of four integer values which indicate the sub-region by column and
* row numbers: column (1) and row (2) numbers of upper left corner and column (3)
* and row (4) number of lower right corner
SUBREG = 1 1 4 4

* Nodes, defined by their column and row numbers, for which pressure head needs to
* be printed to output files (max. 5 nodes, i.e. max. 10 integer values)
HOUT = 1, 1,  3, 6

* Nodes, defined by their column and row numbers, for which water content needs to
* be printed to output files (max. 5 nodes, i.e. max. 10 integer values)
WCOUT = 1, 1,  3, 6
```

15.4.6 Input file WEATHER.DAT

The time-dependent (top) boundary conditions are given in file WNAME (example in Table 15-10). 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 TNAME, the time units for the variables in the file WNAME MUST be equal to that defined in the variable UNITS in file TNAME.

Table 15-10. Example input file WEATHER.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Method for computation of evapotranspiration
*    ETMETH = 0: user supplies RAIN, EPOT, TPOT
*    ETMETH = 1: ET0 according to Penman; supply also: ISURF, RF, TDMI, PENMAN;
*                PENMAN must be either 'PE' (Penman; default) or 'PM' (Penman-
*                Monteith), in the latter case supply also cut-off LAIXDP
*    ETMETH = 2: ET0 according to Priestley-Taylor; supply also : RF
*    ETMETH = 3: ET0 according to Makkink
*    ETMETH = 4: ET0 given as input
* ETMETH = 1,2,3: using routines of van Kraalingen and Stol (1997); see this
* reference for meaning of specific variables
* If ETMETH = 1,2,3  always supply the following data:
*    IFLAG, COUNTR, ISTN, IYEAR, WTRDIR (optional), LOGF (optional)
* which refer to standardized weather files (van Kraalingen et al., 1991)
* There is some consistency check between the use of ETMETH, METHIR and WTYPE:
* illegal: WTYPE = 'Shell' and ETMETH = 1, 2, 3; WTYPE = 'Shell' and METHIR > 0
ETMETH = 0

* Supply the following information depending on the value of METHIR:
*   METHIR = 0      RAIN, TPOT, EPOT
*   METHIR = 1      TPOT, EPOT, IRRINT, LFRAC, ETPTH
*   METHIR = 2      TPOT, EPOT, IRRINT, LFRAC, HTRESH, ITRESH, JTRESH
*   METHIR = 3      TPOT, EPOT, IRRINT, LFRAC, ECTRSH, ITRESH, JTRESH
*
*   IRRINT: irrigation intensity (mm/UNITS)
*   LFRAC : additional fraction of summated evapotranspiration SUMETP that will be
*           supplied as irrigation this is not equal to the well-known leaching
*           fraction LF; LFRAC and LF are related by: LFRAC = LF/(1-LF) or
*                                                     LF = LFRAC/(1+LFRAC)
*   ETPTH : threshold value for summated evapotranspiration SUMETP at which
*           irrigation is initiated
*   HTRESH: threshold value for pressure head at node defined by column ITRESH and
*           row JTRESH at which irrigation is initiated
*   ECTRSH: threshold value for electrical conductivity at node defined by column
*           ITRESH and row JTRESH at which irrigation is initiated

* All variables must be in mm/UNITS, with UNITS defined in file TNAME.
RAIN   = 300*1.0
EPOT   = 300*0.1
TPOT   = 300*0.7
ET0    = 300*0.8

* In case ETMETH = 4 a LAI table must be supplied
*    LAIS   : list of LAI
*    IDOYLAI: list of days
*    IYRLAI : list of years
* Linear interpolation is used for intermediate dates
LAIS  IDOYLAI   IYRLAI
0.0     1        1990
0.0   120        1990
1.0   135        1990
4.0   225        1990
0.0   226        1990
0.0   365        1990

* KCROP: exponential LAI factor
KCROP  = 0.525

* Need crop factor be included (IFCROP = 1) or not (IFCROP = 0; default)
IFCROP = 0
```

```
* In case ETMETH = 4 a FCROP table must be supplied (if IFCROP = 1)
*    FCROPS : list of crop factors
*    IDOYFCR: list of days
*    IYRFCR : list of years
* Linear interpolation is used for intermediate dates
FCROPS  IDOYFCR   IYRFCR
0.0        1      1990
0.0      120      1990
1.0      135      1990
1.1      140      1990
1.1      200      1990
1.0      201      1990
1.0      225      1990
0.0      226      1990
0.0      365      1990

* NB: For both LAI and FCROP the year 1000 may be used as a 'standard' year, i.e.
* for each simulation year one single LAI and/or FCROP sequence can be used
* (instead of supplying the same sequence for each of the years to be simulated.
```

15.4.7 Input file SOILS.DB

The hydraulic parameters should be supplied in a separate file. It is useful to store all available parameters in a single database file (maximum 100 soil types) and store this database at a unique location on the hard disk. Table 15-11 presents an example of such a database file which is self-explanatory.

Table 15-11. Example of the Van Genuchten-Mualem database file.

```
* Database of parameters for the Van Genuchten - Mualem models of the water
* retention and hydraulic conductivity curves.

* TBNAME       name of soil
* TKS          saturated hydraulic conductivity Ks (cm d⁻¹)
* TND          n parameter (drying curve)
* TL           ? parameter
* TALP         a parameter (cm⁻¹)
* TALPD        ad parameter (cm⁻¹)
* TALPW        aw parameter (cm⁻¹)
* TWCS         saturated volumetric water content ?s (-)
* TWCR         residual volumetric water content ?r (-)
* TNW          n parameter (wetting curve, but it is advised to have TNW = TND)
* TKK          K where linear part of hydraulic conductivity changes to the Mualem
*              hydraulic conductivity; when no linear part is present make TKK = TKS
* WCK          q where linear part of hydraulic conductivity changes to the Mualem
*              hydraulic conductivity; when no linear part is present make WCK = WCS

  TBNAME       TKS    TND     TL     TALP   TALPD   TALPW   TWCS  TWCR  TNW    TKK    TWCK
! ------     ------  -----  ------   ------  ------  ------  ----  ----  -----  -----  ----
!
!                           'Staringreeks'; units in 'cm' and 'd'.
!                           (Wösten et al, 1994)
!
!       ALPHAW = 2 * ALPHAD, for the time being
!
!       upper soils ("bovengronden")
'zandb1'     17.46  1.507  -0.140   0.0249  0.0249  0.0498  0.43  0.01  1.507  17.46  0.43
```

```
'zandb2'       9.65  1.548  -0.983  0.0227  0.0227  0.0454  0.43  0.02  1.548   9.65  0.43
'zandb3'      17.81  1.412  -0.213  0.0152  0.0152  0.0304  0.45  0.01  1.412  17.81  0.45
'zandb4'      54.80  1.559   0.177  0.0163  0.0163  0.0326  0.42  0.01  1.559  54.80  0.42
'zavelb7'     14.07  1.250  -0.802  0.0194  0.0194  0.0388  0.40  0.00  1.250  14.07  0.40
'zavelb8'      2.25  1.284  -2.733  0.0096  0.0096  0.0192  0.43  0.00  1.284   2.25  0.43
'zavelb9'      1.54  1.325  -2.161  0.0065  0.0065  0.0130  0.43  0.00  1.325   1.54  0.43
'kleib10'      1.17  1.224  -4.795  0.0118  0.0118  0.0236  0.42  0.01  1.224   1.17  0.42
'kleib11'      5.26  1.111  -5.395  0.0243  0.0243  0.0486  0.60  0.00  1.111   5.26  0.60
'kleib12'     15.46  1.081  -8.823  0.0532  0.0532  0.1064  0.55  0.00  1.081  15.46  0.55
'leemb14'      0.80  1.305   0.000  0.0051  0.0051  0.0102  0.42  0.01  1.305   0.80  0.42
'veenb16'     13.44  1.320   0.534  0.0134  0.0134  0.0268  0.73  0.00  1.320  13.44  0.73
'veenb17'      4.46  1.140  -0.350  0.0180  0.0180  0.0360  0.72  0.00  1.140   4.46  0.72
'veenb18'      6.67  1.154  -1.845  0.0197  0.0197  0.0394  0.77  0.00  1.154   6.67  0.77
!
!      bottom soils ("ondergronden")
'zando1'      13.21  2.167   0.000  0.0224  0.0224  0.0448  0.36  0.01  2.167  13.21  0.36
'zando2'      15.56  2.075   0.039  0.0214  0.0214  0.0428  0.38  0.02  2.075  15.56  0.38
'zando3'      18.30  1.564  -0.522  0.0211  0.0211  0.0422  0.34  0.01  1.564  18.30  0.34
'zando4'      53.10  1.540  -0.520  0.0216  0.0216  0.0432  0.36  0.00  1.540  53.10  0.36
'zando5'      43.55  2.059   0.343  0.0597  0.0597  0.1184  0.32  0.01  2.059  43.55  0.32
'zando6'       5.48  1.152  -6.864  0.0291  0.0291  0.0582  0.41  0.00  1.152   5.48  0.41
'zavelo8'      9.08  1.342  -0.803  0.0136  0.0136  0.0272  0.47  0.00  1.342   9.08  0.47
'zavelo9'      2.23  1.400  -1.382  0.0094  0.0094  0.0188  0.46  0.00  1.400   2.23  0.46
'zavelo10'     2.22  1.280  -2.123  0.0107  0.0107  0.0214  0.49  0.00  1.280   2.22  0.49
'kleio11'     13.79  1.152  -1.384  0.0191  0.0191  0.0382  0.42  0.00  1.152  13.79  0.42
'kleio12'      1.14  1.159  -4.171  0.0095  0.0095  0.0190  0.56  0.00  1.159   1.14  0.56
'kleio13'      3.32  1.110  -4.645  0.0171  0.0171  0.0342  0.57  0.00  1.110   3.32  0.57
'leemo14'      0.36  1.686   0.057  0.0025  0.0025  0.0050  0.38  0.00  1.686   0.36  0.38
'leemo15'      3.70  1.298   0.912  0.0071  0.0071  0.0142  0.41  0.01  1.298   3.70  0.41
'veeno16'      1.07  1.376  -1.411  0.0103  0.0103  0.0206  0.89  0.00  1.376   1.07  0.89
'veeno17'      2.75  1.274  -1.832  0.0127  0.0127  0.0254  0.86  0.00  1.274   2.75  0.86


!
!                      User defined soils; units in 'cm' and 'd',
!
* KIRKLAND ET AL, 1992. Water Resour. Res. 28:2049-2058    (cm/d)
'glendale'   13.1  1.3954  0.5  0.0104  0.0104  0.0208  0.4686  0.106   1.3954  13.1  0.4686
'berino'    541.0  2.239   0.5  0.028   0.028   0.056   0.3658  0.0286  2.239  541.0  0.3658


* HEINEN, 1997. PhD Thesis WAU   (cm/d)
'sandtop'  1256.0  4.98171  0.52581  0.06069  0.06069  0.11745  0.326  0.01573  4.98171  1256.0  0.326
'sandbot'  1256.0  4.90919  0.52581  0.05312  0.05312  0.09466  0.311  0.02311  4.90919  1256.0  0.311


* OTTEN, 1994. PhD Thesis WAU   (cm/d)
'wilfred'  8640.0  1.42   2.35   0.13   0.13   0.90   0.92   0.0  1.42  8640.0  0.92


* KIPP EN WEVER, 1994. PBG Informatiereeks    (cm/d)
'steenwol'  8640.0  4.54872  0.5  0.02572  0.02572  0.05144  0.85  0.0  4.54872  8640.0  0.85
'veenmos'   8640.0  1.425    0.5  0.05964  0.05964  0.11928  0.94  0.0  1.425    8640.0  0.94


* DA SILVA ET AL, 1995. Acta Hortic. 401:71-75.    (cm/d)
'rockwool' 6192. 3.90471 -.28288 .0873 .0873 .55363 .92402 .00673 3.90471  6192.  .92402


* KOOL AND PARKER, 1987. Water Resour. Res. 23:105-114.    (cm/d)
'rubicslm'  25.92  3.301  0.5  0.0136  0.0136  0.0378  0.381  0.17   3.301  25.92  0.381
'guelphl'   31.68  2.14   0.5  0.0098  0.0098  0.0196  0.434  0.219  2.14   31.68  0.434


* Lovinkhoeve; PhD Thesis J.A. de Vos, Table 8.3
'LOV1'  200. 1.30740 -2.02754 0.02190 0.02190 0.04380 0.43709 0.04040 1.30740 200. 0.43709
'LOV2'  200. 1.62422 -1.84898 0.00525 0.00525 0.01050 0.47303 0.08165 1.62422  200. 0.47303
'LOV3'  300. 1.62422 -1.84898 0.00525 0.00525 0.01050 0.47303 0.08165 1.62422  300. 0.47303
'LOV4'  120. 1.91432 -1.46461 0.00207 0.00207 0.00414 0.51506 0.10060 1.91432  120. 0.51506
'LOV5'   40. 1.91432 -1.46461 0.00207 0.00207 0.00414 0.51506 0.10060 1.91432  40. 0.51506
'LOV6'   20. 1.91432 -1.46461 0.00207 0.00207 0.00414 0.51506 0.10060 1.91432  20. 0.51506
'LOV7'   10. 1.91432 -1.46461 0.00207 0.00207 0.00414 0.51506 0.10060 1.91432  10. 0.51506
'LOV8'    2. 1.91432 -1.46461 0.00207 0.00207 0.00414 0.51506 0.10060 1.91432  2. 0.51506
'LOV9'  200. 1.62422 -1.84898 0.00525 0.00525 0.01050 0.47303 0.08165 1.62422  200. 0.47303
```

15.4.8 Input file EXTMAKE.DAT

During initialization of FUSSIM2 a reduction table for evaporation at the soil surface is created. For this purpose the user must supply a range of pressure heads (H) that can be expected to occur for the top layer and a range of potential evaporation rates (ES0) that can be expected (see Table 15-12). For safety reasons these ranges should be large. However, experience shows that for extreme combinations (e.g. low H and high ES0) computations fail, so that the ranges must be decreased.

For practical reasons the file EXTMAKE.DAT must also contain values for NNTAB, PPBIG, PPREF and PPEND. These have the same meaning as those that must be supplied in the file TGEN.DAT (see section 15.4.22) and can have the same values.

Table 15-12. Example of the file EXTMAKE.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Enter a range of pressure heads H (cm)
H = 1.0E20   0.0  -200. -300. -400.  -500. -600. -700. -800. -900. -1000.
      -1500. -2000. -5000. -7500. -10000.

* Enter a range of potential evaporation ESO (cm/d)
ES0 = 0.0  0.005  0.10  0.15  0.20  0.25  0.30  0.35  0.40  0.45  0.50

* to construct intermediate TAB table (see description of TGEN.DAT)
NNTAB =      99
PPBIG = 4000000.
PPREF = 5000000.
PPEND =       0.

* EXTMETHOD: use existing EXT tables or compute EXT tables
*    EXTMETHOD = 'EXISTING'
*    EXTMETHOD = 'COMPUTE'  (default)
EXTMETHOD = 'COMPUTE'

* log progress to screen
SCRNLOG = .FALSE.

* METHOD = 'ONE' : for total range of K integration is used
* METHOD = 'TWO' : for large K integration is used, for small K simple
*                  approximation is used (faster, and difference
*                  with ONE is very small)
METHOD = 'TWO'

* integration method
*    MINT = 'GAUS' : Gaussian integration
*    MINT = 'ROMB' : Romberg integration ; preferred, but slower
MINT = 'ROMB'
```

15.4.9 Input file GWL.DAT

For the special bottom boundary condition IBOT = -4 (see file BOUNDS.DAT) a separate file GWL.DAT must be supplied containing year (IYRGWL), time

(DOYGWL) of measurement of the ground water level (GWLS). GWLS must be in cm below soil surface. The time may (must be a real value) be supplied as fraction of the day, so that the actual time (instead of only day number) of measurement can be used. More than one year can be present. Years must be in ascending order, as well as times within a year. No more than 1000 data can be supplied (maximum 100 years, maximum 400 times per year).

Table 15-13. Example of the file GWL.DAT.

```
* Data of groundwater level (GWLS) in cm below soil surface.
* Time supplied as real DOYGWL and integer IYRGWL; for intermediate dates
* linear interpolation is used.
IYRGWL  DOYGWL      GWLS
1992        1.0     60.0
1992       72.0     30.0
1992       73.0      5.0
1992      281.0     86.0
1992      323.0     28.7
1992      330.0      7.6
1992      337.0      9.8
1992      366.0     30.0

* NB: The year 1000 may be used as a 'standard' year, i.e. for each simulation year
* one single GWL sequence can be used (instead of supplying the same sequence for
* each of the years to be simulated.
```

15.4.10 Input file VIMOKE.DAT

If a Vimoke drain is to be considered the file VIMOKE.DAT must be present with the number of drains NDRAIN = 1. If NDRAIN = 0 no Vimoke drain is considered. At present only a single Vimoke drain can be considered. The location of the drain is given by column and row numbers IDRAIN and JDRAIN.

HDRAIN, IDOYHDRAIN, IYEARHDRAIN
Mostly the outlet of the drain is above the ditch water level. In that case the pressure head of the node of the running Vimoke drain is kept at zero. However, if the outlet is below ditch level, the pressure head of the node representing the Vimoke drain should be equal to the positive difference between ditch level and drain outlet. This difference in pressure is given as HDRAIN and the time is given as year (IYEARHDRAIN) and day (IDOYHDRAIN) number. Linear interpolation is used for intermediate times. Maximum 30 years and 366 day per year can be considered (in total no more than 1000 data). Years and, within years, day number must be in ascending order.

Table 15-14. Example of the file VIMOKE.DAT.

```
* Number of Vimoke drains (0 or 1)
NDRAIN = 1

* Column (IDRAIN) and row (JDRAIN) numbers of Vimoke drain location
IDRAIN = 1*1
JDRAIN = 1*10

* Correction factor CF for parameter CD
CDCORR = 2.0

* Effective drain radius (cm)
REFF = 1.0

* Time table with HDRAIN: H inside drain when functioning. Time is
* specified by IYEAR and IDOY and for intermediate dates linear
* interpolation is used.
* If negative H inside drain becomes zero
HDRAIN    IDOYHDRAIN    IYEARHDRAIN
  -1.0       1            1992
  -1.0      366           1992

* NB: The year 1000 may be used as a 'standard' year, i.e. for each simulation year
* one single HDRAIN sequence can be used (instead of supplying the same sequence
* for each of the years to be simulated.
```

15.4.11 Input file THHFXFZ.DAT

If a steady-state situation for water movement is to be considered, the steady-state distribution of volumetric water content (WC), pressure head (H), water flux density in the x (FX) and z (FZ) direction must be supplied in the file THHFXFZDAT (see Table 15-15).

Table 15-15. 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.

```
* NL*NC values for water content distribution at steady state
WC =
      0.2    0.2    0.25
      0.25   0.25   0.3
      0.3    0.31   0.35
* NL*NC values for pressure head distribution at steady state
H =
      -100.  -100.  -95.
       -95.  -95.   -80.
       -80.  -78.   -50.
* NL*(NC+1) values for horizontal water flux density distribution at steady state
FX =
      0.0    0.0    -0.1   0.0
      0.0    0.0    -0.12  0.0
      0.0    -0.01  -0.2   0.0
* (NL+1)*NC values for vertical water flux density distribution at steady state
FZ =
      -0.05  -0.05  -0.05
      -0.05  -0.05  -0.05
      -0.05  -0.05  -0.05
      -0.05  -0.05  -0.05
```

15.4.12 Input file WET.DAT

In case the variable WET (FUS2.CTR) has the value 'LINEAR' than tabulated wetting data must be supplied in the file WETDAT. This file must contain one series of *x* data (XWET) and NSOILS series of *y* data (YWET), where XWET is the pressure head and YWET is the volumetric water content of the main wetting curve. In the example of Table 15-16 two different soil layers were used, each with a different wetting curve.

Table 15-16. Example of file WET.DAT.

```
XWET =
0.0, 1.0, 2.5, 5.0, 10.0, 15.0, 20.0, 25.0, 30.0, 40.0, 50.0, 60.0, 80.0, 100.0,
10000000.0

YWET =
0.326,   0.326,   0.249,   0.197,   0.141,   0.0945, 0.058, 0.027, 0.0225, 0.0195,
0.0175, 0.017,  0.017,  0.017,  0.01573
0.311,   0.311,   0.244,   0.215,   0.1605, 0.1095, 0.0695, 0.0335, 0.029, 0.027,
0.0235, 0.0235, 0.0235, 0.0235, 0.02311
```

15.4.13 Input file STEMP.DAT

The file STEMPDAT (Table 15-17) contains information for the computation of 1D soil temperature distribution. See chapter 14.

Table 15-17. Example of the file STEMP.DAT.

```
* Annual average T (TYAV) and amplitude of average yearly cycle (TYAMP) (degree C)
TYAV   = 11.4
TYAMP  =  8.9

* Periodic time (TC), initial time (TINI) and time where T=TYAV (TIMAV) (d)
TC     = 365.0
TIMAV  = 121.0
TINI   =   1.0

* Number of time steps to go from TIME1 to TIME2
DTSTEP = 1

* How to compute Ch
*   COMPUTE        (supply also FO per soil layer)
*   INTERPOLATE
CMETH  = 'INTERPOLATE'

* Soil type per layer: either SAND, CLAY or PEAT
* (if you supply only 1 value --> all layers are of the same type)
SOIL   = 1*'SAND'

* How to handle top and bottom boundary condition (COMPUTE or INPUT)
METH1  = 'INPUT'
METHNL = 'COMPUTE'
```

15.4.14 Input file SOLUTE.DAT

The input data for solute transport are given in file SNAME (example in Table 15-18). Additional information for 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).

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.

FREQF   <optional>
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.

Table 15-18. Example input file SOLUTE.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Top boundary condition.
* 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)
* Supply 1 (for all columns the same condition) or NC values
JTOP   = 10*0

* Fixed concentration or concentration during inflow.
* Supply NION*(number of values supplied for JTOP) values.
CTOP   = 10*0.

* Bottom boundary condition.
* 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)
* Supply 1 (for all columns the same condition) or NC values
JBOT   = 10*0

* Fixed concentration or concentration during inflow.
```

```
* When CBOT < 0, inflow occurs with a concentration equal to CONC of the bottommost
* layer.
* Supply NION*(number of values supplied for JBOT) values.
CBOT   = 10*0.

* Left boundary condition.
* 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)
* Supply 1 (for all rows the same condition) or NL values
JLEFT  = 10*0, 16*1

* Fixed concentration or concentration during inflow.
* Supply NION*(number of values supplied for JLEFT) values.
CLEFT  = 26*0.

* Right boundary condition.
* 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)
* Supply 1 (for all rows the same condition) or NL values
JRIGHT = 26*1

* Fixed concentration or concentration during inflow.
* Supply NION*(number of values supplied for JRIGHT) values.
CRIGHT = 26*0.1

* IDISP : method of dispersivities
*    IDISP = 0      use single dispersivity LD
*    IDISP = 1      use longitudinal and transversal dispersivities AL and
*                   AT (default)
IDISP = 1

* Longitudinal dispersion length (cm) (if IDISP = 0; single value)
LD = 10.0

* Longitudinal and transversal dispersivities AL and AT (if IDISP = 1)
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
AL = 1*2.0
AT = 1*0.2

* Three parameters describing two linear parts of the impedance (FIMP) water
* content relationship
*    CF1  : slope
*    CF2  : intercept
*    WCLOW: water content where two linear relationships intersect
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
CF1   = 1*1.58       ! sand or loam (clay: 0.99)
CF2   = 1*-0.17      ! sand, loam, or clay
WCLOW = 1*0.12       ! sand or loam (clay: 0.20)

* Dry bulk density distribution (g/cm3)
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
BDS = 1*1.35
```

```
* parameter ICON determines whether the following table contains initial
* CONCentration (ICON > 0) or AMOUNT (ICON = 0) data
ICON = 1

* Initial distribution of all NION ions.
*     ICON > 0: CONC in mmol/l
*     ICON = 0: AMOUNT in mmol/kg soil
*     ICON < 0; AMOUNT in mgram/kg soil
* Supply NION (all nodes the same value), NION*NL (all nodes per row the same
* value) or NION*NL*NC values (supply a value for each node: first NC values for
* layer 1, second NC values for layer 2, etc.)
CONC   = 1*5.0, 1*0.5
!AMOUNT = 1*20.0, 1*4.0

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

* Frequency of using nutrient solution every irrigation event.
* FREQF = 3 means use nutrient solution every third irrigation event.
FREQF = 1
```

15.4.15 Input file AMMONIUM.DAT

If the file AMMONIUMDAT is supplied and present, ammonium adsorption similar
as described for phosphate (see Chapter 8, but without fixation) can be considered.
See description of file PHOSPHORDAT for additional information.

*15-19. Example of the file AMMONIUM.DAT. Optional variables are printed in italic (see end of section
15.4 for explanation).*

```
* Type of adsorption isotherm:
*     linear     : LINPAR = .TRUE.
*     non-linear: LINPAR = .FALSE.
LINPAR = .FALSE.

* Type of non-linear adsorption isotherm (if LINPAR = .FALSE.)
*     Langmuir   : MODPAR = .TRUE.
*     Freundlich: MODPAR = .FALSE.
MODPAR = .TRUE.

* Constant for linear adsorption AK (ml/cm3) (if LINPAR = .TRUE.)
AK = 2.0

* Langmuir constants (if LINPAR = .FALSE. and MODPAR = .TRUE.)
*     A1, A2 in mg/cm3
*     B1, B2 in ml/mg
* Note that a single (with A2 = B2 = 0) or double Langmuir can be used.
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
B1 = 1*106.8
```

```
B2 = 1*0.0
A1 = 1*0.108
A2 = 1*0.0

* Freundlich constants
*    FREUN: N coefficient of Freundlich isotherm (-)
*    FREUM: M coefficient of Freundlich isotherm (mg/cm3.(mg/ml)^-FREUN)
FREUN = 2.0
FREUM = 1.5

* Desired output
OUTNH4 = 0                ! print NH4 adsorbed distribution
```

15.4.16 Input file IONSINFO.DAT

General information about the ions possibly present in solution is given in the file
IONSINFO.DAT (example in Table 15-20).

Table 15-20. Example input file IONSINFO.DAT.

```
* Information of 13 individual ions, needed for EC computations in SOLUTE
* name, valence, ionic mobility [cm2/(s.V)], diameter [Angstrom = 10^-10 m],
*      diffusion in free water [cm2/d], yes/no consider

* MOBIL must be in units [cm2/(s.V)] ( not using time units d, h, m !!! )
* DIF0 in cm2/d: program converts units corresponding to UNITS as supplied
*      in timer file
* MOLWT: molecular weight (g/mol = mg/mmol)

IONNAM   IONYES   VALENC   MOBIL    IONRAD  DIF0    MOLWT
*************************************************************
'NO3'    1        1        7.41E-4   3.     1.64    14.0067
'K'      1        1        7.62E-4   3.     1.69    39.102
'P'      1        1        3.42E-4   4.     0.759   30.9738
'Ca'     1        2        6.17E-4   6.     0.685   40.08
'Mg'     1        2        5.50E-4   8.     0.610   24.305
'S'      1        2        8.29E-4   4.     0.920   32.064
'Cl'     0        1        7.91E-4   3.     1.76    35.453
'Na'     0        1        5.19E-4   4.     1.15    22.9898
'NH4'    1        1        7.62E-4   3.     1.69    14.0067
'HCO3'   0        1        4.61E-4   4.     1.02    61.01732
'CO3'    0        2        7.64E-4   5.     0.828   60.00935
'H'      0        1        3.63E-3   9.     8.06     1.00797
'OH'     0        1        2.01E-3   3.     4.46    17.00737

* To compute ion activity coefficient, three equations can be used:
*    extended Debye-Huckel (default), approximation for dilute solutions,
*                                   approximation for concentrated solutions
* Variable DEBYE gives method to use
*    DEBYE = 0   default, use extended Debye-Huckel theory)
*          = 1   use approximation for dilute solutions
*          = 2   use approximation for concentrated solutions
*          = 3   use approximations for dilute and/or concentrated solutions
* Of course, approximation are only used when applicable, i.e. a dilute
* solution has I < 0.005, and a concentrated solution has I > 0.1; if not,
* the standard Debye-Huckel 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          ! must be zero
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 Angstrom (10^-10)
```

15.4.17 Input file NITDENIN.DAT

When the module NITDEN is to be considered the file NITDENINDAT must be supplied and present. Table 15-21 presents an example of the file NITDENINDAT as supplied by J.G. Conijn. It describes in detail the meaning of all parameters, and gives (where available) indications of ranges of the values for these parameters.

Table 15-21. Example of input file NITDENIN.DAT. This example was kindly made available by J.G. Conijn.

```
!NITDENIN.DAT: Data input file for NITDEN as used in FUSSIM2/CNGRAS
!****************************************************************

!The data input below has been arranged per type of input data.
!Three types have been distinguished:

!1. State variables.
!The values for the state variables determine the state
!of the model system at the beginning of a simulation run.

!2. Parameters.
!Parameters have a constant value during a simulation run.

!3. Interpolation tables.
!These tables contain pairs of X,Y variables. The Y-value for any X-value
!is found by means of linear interpolation between the two nearest
!X,Y points of the input table.

!Note: NITDEN.F90 and NITDENIN.DAT have been based on earlier work of J.
!      Bril et al., 1994. AB-DLO report 24, pp 21- 25 (see also references below).

! Subroutine : NITDEN (Calculation of (de)nitrification)
!********************************************************

!1. Section NITrification

!1.1 State variables

!Note: pH and CEC are not treated as (state) variables but are assumed
!      constant throughout the whole simulation run. They are read from
!      interpolation tables as function of soil depth (see below)

!1.2 Parameters

NitSourceParam1 = 195.0D0              ! range: [19.5D0, 1950.0D0]
```

```
!NitSourceParam1   parameter used to calculate a multiplication factor which
!                  represents the effect of the ammonium concentration in the
!                  soil on nitrification rate ((mmol NH4)^2 (kg wet soil)^-2 ;
!                  see k2 in equation 8 at page 21)

NitWaterParam1 = 1.2D0                  ! range: [0.6D0 , 3.0D0]
NitWaterParam2 = 1.75D0                 ! range: [0.75D0, 7.0D0]

!NitWaterParam1    first parameter in calculating a multiplication factor
!                  for the effect of water filled pore space on nitrification
!                  rate (- ; see equation 8c at page 22). This parameter
!                  determines the value of the optimum WFPS, where f(WFPS)=1.
!NitWaterParam2    second parameter in calculating a multiplication factor
!                  for the effect of water filled pore space on nitrification
!                  rate (- ; see equation 8c at page 22). This parameter
!                  determines the area underneath the optimum curve.

!Note:  after changing these parameter values a check should be made whether the
!       relation between f(WFPS) and WFPS is still acceptable according to
!       expert judgement.

NitTempParam1   = 3.15D-3               ! range: [,]
NitTempParam2   = 2.0D0                 ! range: [,]
NitTempParam3   = 1.0D-7                ! range: [,]
NitTempParam4   = 5.0D0                 ! range: [,]

!NitTempParam1     first parameter in calculating a multiplication factor
!                   for the effect of soil temperature on nitrification rate
!                   (- ; see equation 8a at page 21).
!NitTempParam2     second parameter in calculating a multiplication factor
!                   for the effect of soil temperature on nitrification rate
!                   (- ; see equation 8a at page 21).
!NitTempParam3     third parameter in calculating a multiplication factor
!                   for the effect of soil temperature on nitrification rate
!                   (- ; see equation 8a at page 21).
!NitTempParam4     fourth parameter in calculating a multiplication factor
!                   for the effect of soil temperature on nitrification rate
!                   (- ; see equation 8a at page 21).

!Note:  after changing these parameter values a check shoud be made whether the
!       relation between f(T) and soil temperature is still acceptable
!       according to expert judgement.

NitpHParam1     = 5.0D+4                ! range: [0.25D+4, 100.0D+4]

!NitpHParam1       parameter in calculating a multiplication factor for the
!                  effect of pH on nitrification rate (- ; see equation 8b at
!                  page 21). This parameter determines the value of the pH,
!                  where f(pH) = 0.5

NitCECParam1    = 20.0D0                ! range: [8.0D0, 50.0D0]
NitCECParam2    =  3.0D0                ! range: [0.0D0, 30.0D0]

!NitCECParam1      first parameter in calculating a multiplication factor
!                  for the effect of CEC on nitrification rate ((mmol NH4)^2
!                  (kg wet soil)^-2 d^-1 ; see equation 8 at page 21).
!                  This parameter equals the value of the multiplication
!                  factor at CEC = 0.
!NitCECParam2      second parameter in calculating a multiplication factor
!                  for the effect of CEC on nitrification rate ((mmol NH4)^2
!                  (kg wet soil)^-2 d^-1 ; see equation 8 at page 21).
!                   This parameter determines the effect of CEC on the multiplication
factor.
```

```
NitPartParam1    = .002D0                    ! range: [0.0D0, 0.05D0]
NitPartParam2    = 0.2D0                     ! range: [0.0D0,(1.0D0-NitPartParam1)]
NitPartParam3    = 0.5D0                     ! range: [0.2D0, 0.8D0]
NitPartParam4    = 3.0D0                     ! range: [1.0D0, 5.0D0]

!NitPartParam1    minimum fraction of total nitrification that is converted
!                 into N2O (- ; see equation 9 at page 23)
!NitPartParam2    maximum fraction of total nitrification that is converted
!                 into N2O (- ; see equation 9 at page 23)
!NitPartParam3    water filled pore space threshold value below which the
!                 effect of WFPS on N2O production from nitrification equals
!                 zero. (- ; see equation 9 at page 23)
!NitPartParam4    fourth parameter to calculate the effect of water filled
!                 pore space on fraction of nitrification converted into N2O
!                 (- ; see equation 9 at page 23). This parameter determines
!                 the steepness of the curve relating the fraction converted
!                 into N2O to WFPS.

!1.3 Interpolation tables

pHDepthTabel     = 0.0,5.5 ,      1000.,5.5
CECDepthTabel    = 0.0,15.0,      1000.,15.0

!pHDepthTabel     table to calculate pH (-) per soil layer as function of
!                 soil depth (cm). This table is only used at initialisation.
!                 Range of X: [0., 1000.] and Y:[3.0, 9.0]
!CECDepthTabel    table to calculate CEC (mmol+/100 g dry soil) per soil
!                 layer as function of soil depth (cm). This table is only used
!                 at initialisation.
!                 Range of X: [0., 1000.] and range of Y depends on soil type:
!                 sand: [1.0, 45.0], clay:[5.0, 60.0] and peat:[40.0, 260.0]


!2. Section DENitrification

!2.1 State variables

!Note: amounts of N2O and N2 are state variables in the subroutine, but they
!      are read from interpolation tables as function of soil depth (see below)

!2.2 Parameters

DenSourceParam1 = 0.008D0                    ! range: [0.0008D0, 0.08D0]

!DenSourceParam1  the amount of source in terms of both NO3 and N2O,
!                 corrected for their electron-equivalents, at which
!                 the denitrification rate equals half its maximum rate at
!                 optimal conditions for denitrification (mol NO3/kg moist
!                 soil ; see equation 10 at page 23).
!                 This parameter is the half-value constant in a Monod function.

DenWaterParam1  = 0.5D0!0.3D0               ! range: [0.2D0, 0.8D0]
DenWaterParam2  = 2.5D0                     ! range: [1.0D0, 5.0D0]

!DenWaterParam1   water filled pore space threshold value below which
!                 the denitrification rate equals zero (- ; see equation 10 at
!                 page 23 and page 20)
!DenWaterParam2   second parameter to calculate the effect of water filled
!                 pore space on denitrification rate (- ; see equation 10 at
!                 page 23 and page 20). This parameter determines the
!                 steepness of the curve relating denitrification rate to WFPS.
```

```
DenTempParam1    = 3.76D-3               ! range: [,]
DenTempParam2    = 1.75D0                ! range: [,]
DenTempParam3    = 6.0D-7                ! range: [,]
DenTempParam4    = 4.0D0                 ! range: [,]

!DenTempParam1      first parameter in calculating a multiplication factor
!                   for the effect of soil temperature on denitrification rate
!                   (- ; see f(T)2 at page 19).
!DenTempParam2      second parameter in calculating a multiplication factor
!                   for the effect of soil temperature on denitrification rate
!                   (- ; see f(T)2 at page 19).
!DenTempParam3      third parameter in calculating a multiplication factor
!                   for the effect of soil temperature on denitrification rate
!                   (- ; see f(T)2 at page 19).
!DenTempParam4      fourth parameter in calculating a multiplication factor
!                   for the effect of soil temperature on denitrification rate
!                   (- ; see f(T)2 at page 19).
!Note:   after changing these parameter values a check should be made whether the
!        relation between f(T) and soil temperature is still acceptable
!        according to expert judgement.

DenElectrParam1 = 1.0D+3!5.0D+3         ! range: [0.1D+3, 100.0D+3]
DenpHParam1      = 6.5D0                 ! range: [4.0D0, 9.0D0]
DenpHParam2      = 3.0D0                 ! range: [1.0D0, 9.0D0]
DenpHParam3      = 0.25D0                ! range: [0.0D0, 1.0D0]

!DenElectrParam1   factor for the sink strength of N2O in consuming electrons
!                  relative to that of NO3 at a pH value equal to DenpHParam1
!                  (- ; compare Kb/Ka in equations 11a and 11b at page 24)
!DenpHParam1       pH value at which the factor for the sink strength of N2O in
!                  consuming electrons relative to that of NO3 equals
!                  DenElectrParam1 (- ; see equation 11d at page 24)
!DenpHParam2       second parameter for calculating a multiplication factor
!                  for the effect of pH on the sink strength of N2O in
!                  consuming electrons relative to that of NO3 (- ; see
!                  equation 11d at page 24)
!DenpHParam3       minimum value for the multiplication factor for the effect
!                  of pH on the sink strength of N2O in consuming electrons
!                  relative to that of NO3 (-)

DenEmisParam1    = 0.5D0                 ! range: [0.2D0, 0.8D0]
DenEmisParam2    = 5.0D0                 ! range: [1.0D0, 10.0D0]
DenEmisParam3    = 0.33D0!0.5D0          ! range: [0.1D0, 0.9D0]
DenEmisParam4    = 10.0D0                ! range: [1.0D0, 100.D0]

!DenEmisParam1     water filled pore space value at which the emission fraction
!                  equals half of its maximum value of DenEmisParam3 (cm3/cm3)
!DenEmisParam2     shape parameter for the function relating the emission
!                  fraction to water filled pore space (-)
!DenEmisParam3     maximum fraction of the difference in N2O concentration
!                  between soil air and atmosphere that leaves the soil
!                  as N2O emission at a WFPS value of zero (d^-1)
!DenEmisParam4     parameter used in calculating the N2O concentration in
!                  soil air by partitioning of total N2O between soil water
!                  and soil air as a function of water filled pore space (-)

N2OinAtmosphere = 0.3D0                  ! range: [0.2D0, 0.4D0]
GasConstant     = 22.4D0                 ! 'physical' constant

!N2OinAtmosphere   N-N2O concentration in the atmosphere (ppm)
!GasConstant       gas constant (dm3/mol)

!2.3 Interpolation tables
```

```
!DNPDepthTabel = 0.0,5.0,       1000.,5.0
N2ODepthTabel = 0.0,0.75E-7, 1000.,0.75E-7
N2DepthTabel  = 0.0,0.2,     1000.,0.2

!DNPDepthTabel    table to calculate denitrification potential
!                 (mg N (kg dry soil)^-1 d^-1) per soil layer as function of
!                 soil depth (cm). This table is only used at initialisation.
!                 Range of X: [0., 1000.] and range of Y depends on soil type:
!                 sand: [0.0, 50.0], clay:[0.0, 80.0] and peat:[0.0, 200.0]
!                 (see below for values taken from G.L. Velthof)
!N2ODepthTabel    table to calculate amount of N2O (mg/cm3) per soil layer as
!                 function of soil depth (cm). This table is only used at
!                 initialisation.
!                 Range of X: [0., 1000.] and Y: [0.75E-10, 0.75E-4]
!N2DepthTabel     table to calculate amount of N2 (mg/cm3) per soil layer as
!                 function of soil depth (cm). This table is only used at
!                 initialisation.
!                 Range of X: [0., 1000.] and Y: [0.02, 2.0]

!*********************************************************************
!Data from G.L. Velthof (source: Nitrous oxide emissions from intensively
!managed grasslands ; 1997 ; page 35 (Phd thesis)

!Note: first data point and data beyond layer 40 - 60 cm have been estimated
!      by JGConijn (1st and 3rd line) !!

!Sand
DNPDepthTabel = 0.0, 24.5,
                2.5, 19.0, 7.5, 8.0, 15.0, 3.0, 30.0, 4.0, 50., 0.0,
                70.,0.0, 1000.,0.0
!Clay
!DNPDepthTabel = 0.0, 30.0,
!                2.5, 30.0, 7.5, 6.0, 15.0, 4.0, 30.0, 2.0, 50., 1.0,
!                70.,0.0, 1000.,0.0
!Peat I
!DNPDepthTabel = 0.0,103.0,
!                2.5,103.0, 7.5,30.0, 15.0,13.0, 30.0,12.0, 50.,13.0,
!                70., 6.0, 90.,0.0, 1000.,0.0
!Peat II
!DNPDepthTabel = 0.0, 87.0,
!                2.5, 87.0, 7.5,37.0, 15.0,12.0, 30.0, 4.0, 50., 5.0,
!                70.,0.0, 1000.,0.0
!*********************************************************************

!*********************************************************************
!Data from B. Rutgers (source: zwarte multomap in zijn kast: 'Berekening
!D1 CEC bepaling ...' ; 1987)

!Note: only one value per soil column is measured ; thickness of soil
!      layer not given ; for 3 soil types two methods of analysis have
!      been used: 1 = NH4 & Ca, 2 = Ba & Mg

!Sand Droevendaal (method 1)
!CECDepthTabel = 0.0, 7.2, 1000., 7.2
!Sand Droevendaal (method 2)
!CECDepthTabel = 0.0,16.3, 1000.,16.3

!Sand Achterberg (method 1)
!CECDepthTabel = 0.0, 3.7, 1000., 3.7
!Sand Achterberg (method 2)
!CECDepthTabel = 0.0,12.7, 1000.,12.7
```

```
!Clay Minderhoudhoeve (method 1: not suited due to high Ca in clay)
!
!Clay Minderhoudhoeve (method 2)
!CECDepthTabel = 0.0,21.2, 1000.,21.2

!Peat Zegveld (method 1)
!CECDepthTabel = 0.0, 71.1, 1000., 71.1
!Peat Zegveld (method 2)
!CECDepthTabel = 0.0,130.0, 1000.,130.0
```

15.4.18 Input file PHOSPHOR.DAT

When the file PHOSPHORDAT is supplied and present and when P is present in
the soil solution (IONYES(P) = 1 in IONSINFODAT) P adsorption and fixation is
considered as described in chapter 8. Table 15-22 presents an example of the file
PHOSPHORDAT.

MODPAR, LINPAR
Type of adsorption isotherm is given by the logical MODPAR: TRUE -> Langmuir
(supply A1, A2, B1, B2), else Freundlich (supply FREUN, FREUM). Non-linear
adsorption is considered when LINPAR = FALSE. For LINPAR = TRUE linear
adsorption can be considered (supply AK).

Table 15-22. Example of file PHOSPHOR.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Type of adsorption isotherm:
*    linear    : LINPAR = .TRUE.
*    non-linear: LINPAR = .FALSE.
LINPAR = .FALSE.

* Type of non-linear adsorption isotherm (if LINPAR = .FALSE.)
*    Langmuir  : MODPAR = .TRUE.
*    Freundlich: MODPAR = .FALSE.
MODPAR = .TRUE.

* Constant for linear adsorption AK (ml/cm3) (if LINPAR = .TRUE.)
AK = 2.0

* Langmuir constants (if LINPAR = .FALSE. and MODPAR = .TRUE.)
*    A1, A2 in mg/cm3
*    B1, B2 in ml/mg
* Note that a single (with A2 = B2 = 0) or double Langmuir can be used.
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
B1 = 1*106.8
B2 = 1*0.0
A1 = 1*0.108
A2 = 1*0.0

* Freundlich constants
*    FREUN: N coefficient of Freundlich isotherm (-)
*    FREUM: M coefficient of Freundlich isotherm (mg/cm3.(mg/ml)^-FREUN)
FREUN = 2.0
```

```
FREUM = 1.5

* Initial Pw distribution (mg P2O5 / L soil)
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
PW = 1*10.0

* Fixation rate parameters (Schoumans model, Rapport 381, 1995, SC-DLO)
*    ALPH1,ALPH2,ALPH3  extinction coefficients (1/d)
*    N1,N2,N3           exponents (-)
*    BI1,BI2,BI3        b-parameters (mg P/l)**Ni (Ni=N1,N2 or N3)
*    ALFEOX             oxalate extractable Fe+Al (mmol/kg)
*    REDF               reduction of rate when de-fixation occurs (-)
* Supply 1 (all nodes the same value), NL (all nodes per row the same value) or
* NL*NC values (supply a value for each node: first NC values for layer 1, second
* NC values for layer 2, etc.)
ALPH1  =    1*1.1755
ALPH2  =    1*0.0334
ALPH3  =    1*0.0014382
N1     =    1*0.5357
N2     =    1*0.1995
N3     =    1*0.2604
BI1    =    1*0.009459
BI2    =    1*0.03795
BI3    =    1*0.05185
ALFEOX = 1*210.0
REDF   = 1*100.0

* Desired output
OUTADS = 0                  ! print Pw distribution
         0                  ! print P adsorbed
         0                  ! print P fixated
         0                  ! print P fixing capacity and fraction of P capacity
                            ! occupied
```

15.4.19 Input file UPTA.DAT

Data file for root solute uptake are given in the file UPTA.DAT (example in Table 15-23).

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 15-23. Example input file UPTA.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Maximum uptake rate of nutrient per unit root surface area (De Willigen & van
* Noordwijk 1987, PhD Thesis WAU, p. 48) (mmol/(cm2.day).
* Program converts units corresponding to UNITS as supplied in timer file values
* for all NION ions must be given.
FMAX   = 13*6.05E-04

* Which uptake routine to use
*     IUPWAY = 1: use root nutrient uptake model (default)
*     IUPWAY = 0: consider root nutrient uptake proportional to root length
IUPWAY = 1

* Method how to treat nutrient transport after unconstrained uptake
*     METHOD = 0: diffusion only
*            > 0: mass flow via Eq. [46] and G-function (Eq. [48]) plus diffusion
*            < 0: mass flow as water uptake times concentration plus diffusion
METHODU = 1

* Minimum concentration at root surface below which uptake cannot occur (default is
* zero).
* Supply NION values.
CMIN = 1*0.0

* Maximum number of iterations allowed during uptake distribution computations
IUPMAX = 50

* Convergence criterion for uptake distribution computations
UPCRIT = 1.0E-04
```

15.4.20 Input file TRANSP.DAT

Input data for the root water uptake module are given in the file TRANSP (example in Table 15-24).

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. Logistic
root growth is described by (Heinen, 1997; TIME t is the current simulation time)

$$L_{rv} = \frac{L_{rv,ini}}{1 + \exp\left(-L_{rv,k}\left(t + L_{rv,ts} - L_{rv,t}\right)\right)}$$

When RTGROW = 1, the user should supply the following data.

LRVK   the inverse time constant (d^{-1})

LRVT   the time of inflection of the logistic curve (d)

LRVTS   start time of simulation relative to start of plant growth, i.e. the age of the roots at start of simulation (d)

LRVINI the maximum (asymptotic) root length density distribution

Table 15-24. Example input file TRANSP.DAT. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* Solute reflection coefficient for water uptake model (-).
* Supply 1 (for all plants the same) or NPLANT values.
SIGMA = 1*0.9

* Osmotic pressure head inside plant for water uptake model (cm).
* Supply 1 (for all plants the same) or NPLANT values.
HOSP = 1*0.

* Root hydraulic conductance K1 (cm/d).
* Program converts units corresponding to UNITS as supplied in timer file.
* Supply 1 (for all plants the same) or NPLANT values.
K1 = 1*3.6D-06

* Root radius R0 (cm).
* Supply 1 (for all plants the same) or NPLANT values.
R0 = 1*0.017

* Campbell reduction function parameters (if REDPOT > 0)
*    A    : some plant specific parameter (-)
*    HRHALF: plant potential where reduction function equals 0.5 (cm)
* Supply 1 (for all plants the same) or NPLANT values.
A      = 1*10.0
HRHALF = 1*1.0D4

* Indicate which variables have to be printed
OUTTRA = 0,          ! print root water uptake rate (cm/UNITS) and cumulative root
                     ! water uptake since start (cm): 1: yes, else no
         0,          ! print root water uptake rate per cm root length
                     ! (cm3/(cm root.UNITS)): idem
         0,          ! print relative contribution of root water uptake in relation
                     ! to actual transpiration rate (-): idem
         1,          ! 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

* Reduction parameter REDPOT
*    REDPOT = 0: no transpiration reduction
*    REDPOT = 1: reduction of transpiration according to Campbell reduction
*               function (default)
REDPOT = 1

* Consider logistic root growth (RTGROW = 1) or not (RTGROW = 0; default)
* If RTGROW then supply
*    LRVINI: maximum LRV distribution (NPLANT*NL*NC values)
*    LRVK  : k-parameter in logistic growth function (1 or NPLANT values)
*    LRVT  : time of inflection in logistic growth function (1 or NPLANT values)
*    LRVTS : start time of simulation, i.e. time to be added to simulation time in
*            order to get real time to be used in logistic growth function (1 or
*            NPLANT values)
RTGROW = 0
```

15.4.21 Input file TRANSP.CTR

In the file TRANSP.CTR some control parameters are given used in the root water uptake module (example in Table 15-25).

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 15-25. Example input file TRANSP.CTR. Optional variables are printed in italic (see end of section 15.4 for explanation).

```
* increase/reduction factor for finding proper minimum and maximum values for root
* pressure head
FAC    = 1.25

* convergence criterion root water uptake
RDPMIN = 1.0E-4

* number of points used for interpolation in matric flux potential table
NP     = 3

* accuracy used for root finding procedure
TOL    = 1.0E-4

* Method of transpiration computation.
*    TRANS = 'COMPUTE' : use water uptake model (default)
*    TRANS = 'PROPORT' : water uptake is proportional to root length
TRANS  = 'COMPUTE'

*Yes or No use hysteretic approximation in TRANS (do not change)
TRHYST = 'N'
```

15.4.22 Input file TGEN.DAT

The file TGEN.DAT contains some parameters used by the root water uptake module (example in Table 15-26). 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. In the program the pressure head h is replaced by pressure P with $P = -h$. 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 for which the table is to be constructed 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 15-26. Example input file TGEN.DAT.

```
NNTAB =      99
PPBIG = 100000.
PPREF = 600000.
PPEND =      0.
```

15.4.23 Input file EXPLIN.DAT

When the internal expo-linear plant growth module is to be used (ELGROW = TRUE in FUS2.CTR) the required data must be supplied in the data file EXPLIN.DAT (see Table 15-27). In this same file also data need to be supplied when the internal nutrient demand function is to be considered (NUTDEM = TRUE in FUS2.CTR). See descriptions of these modules in chapter 11.

PLNUM
It is possible to consider more than 1 plant. To distinguish the regions that each plant type occupies, the user must supply per column what plant type PLNUM is growing there. So values for PLNUM must be in the range 1 through NPLANT

Table 15-27. Example input file EXPLIN.DAT.

```
* Number of plants to consider
NPLANT = 1

* Indicate what plant number is coupled to each of the columns
* Enter 1 or NC values
PLNUM  = 1*1

* Parameters for the expo-linear growth equation
*    RM   (g/g/d)  : maximum relative growth rate
*    CM   (kg/ha/d): maximum growth rate
*    WTOT (kg/ha)  : initial dry weight of species
*    SHRT (-)      : shoot-root ratio
*    PL   (g/g)    : fraction of total dry matter that are leafs
*    SLA  (ha/kg)  : specific leaf area
* Enter NPLANT values per variable.
RM     = 1*0.14      ! faba bean
CM     = 1*200.0
WTOT   = 1*50.0
SHRT   = 1*10.0
PL     = 1*0.5
SLA    = 1*200.E-5   ! specific leaf area 200 cm2/g = 200E-5 ha/kg

* Parameters for demand computation
* Maximum uptake rate of nutrient per unit root surface area (p. 48 dW + vN,
* dissertation) (mmol/(cm2.day))
* Program converts units corresponding to UNITS as supplied in timer file
* Enter NPLANT*NION values
```

```
FMAX    = 2*6.05E-4

* Initial amount in plants (kg/ha)
* Enter NPLANT*NION values
TUPT = 2*0.1

* Indicate how the demand is to be computed.
*    DEMMOD = FALSE: use GREENWOOD formula, and additionally supply A, B, C
*    DEMMOD = TRUE:  do interpolation from table, and additionally supply DM and
*                    OPTC tables
DEMMOD = .FALSE.

* Greenwood parameters (if DEMMOD = FALSE)
* A,B in g/g; C in ha/kg
* Enter NPLANT*NION values
A    = 2*0.0021
B    = 2*0.00168
C    = 2*0.00026

* Interpolation table (if DEMMOD = TRUE)
*    DM:   dry matter content of a plant (no more than 10 values; g).
*          Note that only 1 list of DM for all plants can be used.
*    OPTC: list of optimal concentrations of ions in plant (g nutrient / g plant).
*          Enter NDM*NPLANT*NION values, with NDM is the number of DM data.
DM   = 0.0   1.0   10.0   100.0   250.0
OPTC = 0.04, 0.04,  0.035,  0.03,   0.03
       0.02, 0.02,  0.02,   0.02,   0.02

* Relaxation time constant TCNU (d)
* Enter NPLANT*NION values
TCNU = 2*1.0
```

15.4.24 Input file ROOTS.DAT

When diffusive root growth needs to be considered (RGROW = TRUE in FUS2.CTR) the required data must be supplied in the file ROOTSDAT (see Table 15-28).

QIN
Input of roots is presumed to occur at the bottom of the stem of the plant. The user can indicate where this occurs by supplying QIN = 1 for those control volumes, otherwise supply QIN = 0.

Table 15-28. Example input file ROOTS.DAT.

```
* Root radius (cm)
R0     = 1*0.01

* Dry matter content of roots (g/g)
DMCR   = 1*0.08

* Bulk density of roots (g/cm3)
RHOR   = 1*1.0

* Basic diffusion coefficient for root growth in x-direction (cm2/d) (units are
* automatically converted to program time units)
RDX0   = 1*1.0

* Basic diffusion coefficient for root growth in z-direction (cm2/d) (units are
* automatically converted to program time units)
RDZ0   = 1*2.0

* Specific decay rate of roots (1/d) (units are automatically converted to program
* time units)
DECRAT = 1*0.02

* CV's where roots enter from the stem into the substrate (no dimension)
*    QIN = 0: no root input
*    QIN = 1: root input
* Enter NPLANT*NL*NC values
QIN =
      19*0, 1
      19*0, 1
      19*0, 1
      19*0, 1
      20*0,
      120*0

* Initial distribution of LRV (cm/cm3)
* Enter NPLANT*NL*NC values
LRVINI =
      19*0.0, 2.0
      19*0.0, 2.0
      19*0.0, 2.0
      19*0.0, 2.0
      20*0.0,
      120*0.0

* Reduction function for hindering root growth.
* Enter precisely 6 (X,Y) pairs, with
*    X = pressure head (cm)
*    Y = reduction (no dimension)
* Y = 1 no reduction, Y = 0 no root growth; linear interpolation is done for
* intermediate values of X.
REDH  = -100000.0,  0.0,
         -10000.0,  0.0,
          -1000.0,  1.0,
            -10.0,  1.0,
              0.0,  0.0,
           1000.0,  0.0
```

15.4.25 Input file FERTIL.DAT

If the file FERTILDAT is supplied and it exists, then fertilization takes place. In this file (Table 15-29) the times of fertilization (FERTTM) are given as well as the corresponding amount for all ions (FFERT). Also present must be the column and row numbers of all nodes where fertilization takes place.

Table 15-29. Example of file FERTIL.DAT.

```
* Times of fertilization (in time units) (max. 10 values)
FERTTM = 100.0, 130.0, 180.0, 200.0, 225.0

* Amounts of fertilizers (kg/ha) for all NION ions at all FERTTM
FFERT =
 30.0  10.0
 35.0  15.0
 30.0  10.0
 35.0  15.0
100.0  25.0


* Column numbers (FCOL) and row numbers (FROW) where fertilizer is applied (max. 50
* values per array)
FCOL = 1 2 3 4 5 6 7 8 9 10
FROW = 10*1
```

15.5 Examples of output files

A simulation run results in one or two user-supplied output files (RNAME and SNAME, see Section 15.4), a logfile (FUSSIM2.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 FUSSIM2.LOG contains some messages from the TTUTIL 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 15-30); solute results are printed to the user-supplied file SNAME (example in Table 15-31). Examples of these two files are given below, and should be self-explanatory.

Table 15-30. Example of water results file RNAME.

```
         Example 6.4

         Units of measure:
                 Length in : cm   (default).
                 Time in    : d (user supplied).

         Ouput filename                        : c-w
         Soil conditions file name             : c-so
         Boundary and initial conditions filename : c-bc
         Weather conditions filename           : c-wh
         Timer data filename                   : c-tm

         GEOMETRY
         Profile width (cm)          :   200.00
         Profile depth (cm)          :   200.00
         Number of grid points in x :    20
         Number of grid points in z :    24

         Position gridpoints
         X-coordinate gridpoints (cm)
   .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
         Z-coordinates gridpoints (cm)
   .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  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
                                   xN11-
                                  xN1111-
                                 xN111111-
                                x11111111-
                          sNNNNNN111111111-
                          s111111111111111-
                          s111111111111111-
                          s111111111111111-
                          s111111111111111-
                          s111111111111111-
                          s111111111111111-
                          s111111111111111-
                          s111111111111111-
                          h111111111111111-
                          h111111111111111-
                       xhh111111111111111-
                       -111111111111111111-
                       -111111111111111111-
                       -111111111111111111-
                       -111111111111111111-
                       -111111111111111111-
                       -111111111111111111-
                       x-----------------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 EPSILI =    1.00000E-08


        Hydraulic properties for each of the control volumes.


        van Genuchten functions used.


        Averaging hydraulic conductivities : geometric


        No hysteresis considered.


        ICCG0 solution method used.


        No theoretical root water uptake considered.



        TIME =  0.00000000E+00


        Total water          :       1.5558535348E+04 ml
        Total change water :       0.0000000000E+00 ml
        Balance water      :       0.0000000000E+00 ml
        Relative water     :       0.0000000000E+00

        Water content (-)
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-
01  4.00000E-01  4.00000E-01  3.15234E-01  3.15234E-01  3.15234E-01
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-
01  3.23985E-01  3.23985E-01  3.23985E-01  3.23985E-01  3.23985E-01
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  3.30470E-01  3.30470E-
01  3.30470E-01  3.30470E-01  3.30470E-01  3.30470E-01
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  3.37563E-01  3.37563E-01  3.37563E-01  3.37563E-01  3.37563E-01  3.37563E-01  3.37563E-01  3.37563E-01  3.37563E-01
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  3.45352E-01  3.45352E-01  3.45352E-01  3.45352E-01  3.45352E-01  3.45352E-01  3.45352E-01  3.45352E-01  3.45352E-01
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01  3.53928E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01  3.63373E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01  3.73715E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01  3.84800E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01  3.91536E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01  3.93713E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01  3.95805E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01  3.97752E-01
 4.00000E-01  4.00000E-01  4.00000E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01  3.99423E-01
 4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
```

```
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01  4.00000E-01
```

Pressure head (cm)
```
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 -1.00000E+02 -1.00000E+02 -1.00000E+02
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 -8.50000E+01 -8.50000E+01 -8.50000E+01 -8.50000E+01 -8.50000E+01
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 -7.50000E+01 -7.50000E+01 -7.50000E+01 -7.50000E+01 -7.50000E+01 -7.50000E+01
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 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01 -6.50000E+01
0.00000E+00  0.00000E+00  0.00000E+00 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01 -4.50000E+01
0.00000E+00  0.00000E+00  0.00000E+00 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01 -3.50000E+01
0.00000E+00  0.00000E+00  0.00000E+00 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01 -2.50000E+01
0.00000E+00  0.00000E+00  0.00000E+00 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01 -1.50000E+01
0.00000E+00  0.00000E+00  0.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00 -9.00000E+00
0.00000E+00  0.00000E+00  0.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00 -7.00000E+00
0.00000E+00  0.00000E+00  0.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00 -5.00000E+00
0.00000E+00  0.00000E+00  0.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00 -3.00000E+00
0.00000E+00  0.00000E+00  0.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00 -1.00000E+00
0.00000E+00  0.00000E+00  0.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00  5.00000E+00
0.00000E+00  0.00000E+00  0.00000E+00  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01  1.50000E+01
2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01  2.50000E+01
3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01  3.50000E+01
4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01  4.50000E+01
5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01  5.50000E+01
6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01  6.50000E+01
7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01  7.50000E+01
8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01  8.50000E+01
1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02  1.00000E+02
```

Fluxes in x-dir. (cm3/(cm2.t))
```
0.00000E+00  ...  (numeric array)
```

Fluxes in z-dir. (cm3/(cm2.t))
```
0.00000E+00  ...  (numeric array)
```

```
Net total flow into flow domain      :      4.0000000000E+02 ml/d
Total amount that passed top layer   :      4.0000000000E-03 ml
```

```
        Total amount that passed bottom layer   :      0.0000000000E+00 ml
        Total amount that passed left boundary  :      3.7490011096E-19 ml
        Total amount that passed right boundary :      0.0000000000E+00 ml



        TIME =  1.00000000E+01


        Total water           :       1.5964384250E+04 ml
        Total change water :       4.0595898950E+02 ml
        Balance water        :      -1.1008670507E-01 ml
        Relative water       :      -6.8957689405E-06
```

Water content (-)

```
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 3.94572E-01 3.94572E-01 3.94572E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 3.94583E-01 3.94583E-01 3.94583E-01 3.94583E-01 3.94583E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 3.94609E-01 3.94612E-01 3.94613E-01 3.94614E-01 3.94614E-01 3.94615E-01 3.94614E-01 3.94614E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 3.94666E-01 3.94678E-01 3.94692E-01 3.94702E-01 3.94709E-01 3.94713E-01 3.94713E-01 3.94711E-01 3.94708E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.85437E-01 3.91892E-01 3.93744E-01 3.94446E-01 3.94766E-01 3.94915E-01 3.94989E-01 3.95178E-01 3.95394E-01 3.95603E-01 3.95777E-01 3.95904E-01 3.95977E-01 3.95999E-01 3.95977E-01 3.95930E-01 3.95866E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.89667E-01 3.92293E-01 3.93941E-01 3.94894E-01 3.95499E-01 3.95780E-01 3.95630E-01 3.96290E-01 3.97087E-01 3.97829E-01 3.98458E-01 3.98960E-01 3.99337E-01 3.99602E-01 3.99773E-01 3.99869E-01 3.99930E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.92760E-01 3.94153E-01 3.95400E-01 3.96707E-01 3.98269E-01 3.99563E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.96434E-01 3.98131E-01 3.99945E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.98060E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.98666E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.99153E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 3.99513E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01 4.00000E-01
```

Pressure head (cm)

```
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 -6.19094E+00 -6.19095E+00 -6.19096E+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 -6.18038E+00 -6.18023E+00 -6.18017E+00 -6.18020E+00 -6.18030E+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 -6.15511E+00 -6.15318E+00 -6.15139E+00 -6.15045E+00 -6.15023E+00 -6.15047E+00 -6.15098E+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 -5.97526E+00 -5.92817E+00 -5.87561E+00 -5.82768E+00 -5.79119E+00 -5.76866E+00 -5.76003E+00 -5.76275E+00 -5.77180E+00 -5.78499E+00
0.00000E+00 0.00000E+00 0.00000E+00 -1.44366E+01 -8.67679E+00 -6.97099E+00 -6.30992E+00 -6.00643E+00 -5.79241E+00 -5.61035E+00 -5.40098E+00 -5.02713E+00 -4.90218E+00 -4.82949E+00 -4.80833E+00 -4.83011E+00 -4.87603E+00 -4.93977E+00
0.00000E+00 0.00000E+00 0.00000E+00 -1.06817E+01 -8.31073E+00 -6.78624E+00 -5.88377E+00 -5.29912E+00 -5.02410E+00 -5.17105E+00 -4.51848E+00 -3.70534E+00 -2.91548E+00 -2.20887E+00 -1.60741E+00 -1.11839E+00 -7.41885E-01 -4.73229E-01 -3.03905E-01 -1.85544E-01
0.00000E+00 0.00000E+00 0.00000E+00 -7.88291E+00 -6.58730E+00 -5.39590E+00 -4.09695E+00 -2.42554E+00 -8.00354E-01 4.24095E-01 1.50384E+00 2.61224E+00 3.65116E+00 4.58166E+00 5.38785E+00 6.06357E+00 6.60689E+00 7.01740E+00 7.29426E+00 7.50525E+00
0.00000E+00 0.00000E+00 0.00000E+00 -4.37306E+00 -2.58148E+00 -1.51976E-01 2.05812E+00 4.16494E+00 6.25440E+00 8.17584E+00 9.63491E+00 1.08669E+01 1.19876E+01 1.29484E+01 1.37711E+01 1.44565E+01 1.50052E+01 1.54176E+01 1.56937E+01 1.59021E+01
0.00000E+00 0.00000E+00 0.00000E+00 -1.96502E+00 1.75805E+00 5.24605E+00 8.29446E+00 1.07226E+01 1.28724E+01 1.47615E+01 1.63146E+01 1.76346E+01 1.87750E+01 1.97580E+01 2.05934E+01 2.12859E+01 2.18383E+01 2.22523E+01 2.25286E+01 2.27363E+01
0.00000E+00 0.00000E+00 0.00000E+00 -1.36162E+00 3.25159E+00 6.81956E+00 9.89828E+00 1.23800E+01 1.45446E+01 1.64322E+01 1.80007E+01 1.93339E+01 2.04827E+01 2.14707E+01 2.23089E+01 2.30030E+01 2.35562E+01 2.39706E+01 2.42469E+01 2.44545E+01
0.00000E+00 0.00000E+00 0.00000E+00 -8.72658E-01 4.71280E+00 8.41264E+00 1.15260E+01 1.40500E+01 1.62278E+01 1.81157E+01 1.96962E+01 2.10406E+01 2.21968E+01 2.31893E+01 2.40302E+01 2.47257E+01 2.52798E+01 2.56944E+01 2.59708E+01 2.61783E+01
0.00000E+00 0.00000E+00 0.00000E+00 5.00000E+00 6.16902E+00 1.00292E+01 1.31773E+01 1.57339E+01 1.79226E+01 1.98114E+01 2.14012E+01 2.27548E+01 2.39175E+01 2.49141E+01 2.57572E+01 2.64541E+01 2.70088E+01 2.74238E+01 2.77002E+01 2.79076E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.08147E+01 1.49643E+01 1.82021E+01 2.08298E+01 2.30431E+01 2.49345E+01 2.65445E+01 2.79203E+01 2.90996E+01 3.01067E+01 3.09561E+01 3.16564E+01 3.22129E+01 3.26285E+01 3.29050E+01 3.31121E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.50000E+01 2.02228E+01 2.41011E+01 2.71869E+01 2.97374E+01 3.18990E+01 3.37543E+01 3.53509E+01 3.67261E+01 3.79086E+01 3.89187E+01 3.97698E+01 4.04708E+01 4.10271E+01 4.14422E+01 4.17180E+01 4.19244E+01
2.50000E+01 2.50000E+01 2.50000E+01 2.76699E+01 3.09755E+01 3.40303E+01 3.67070E+01 3.90337E+01 4.10614E+01 4.28326E+01 4.43788E+01 4.57247E+01 4.68901E+01 4.78896E+01 4.87338E+01 4.94299E+01 4.99826E+01 5.03951E+01 5.06692E+01 5.08742E+01
3.69471E+01 3.72923E+01 3.79702E+01 3.97040E+01 4.19791E+01 4.43377E+01 4.65772E+01 4.86291E+01 5.04803E+01 5.21361E+01 5.36068E+01 5.49038E+01 5.60373E+01 5.70158E+01 5.78459E+01 5.85323E+01 5.90784E+01 5.94864E+01 5.97577E+01 5.99608E+01
4.86640E+01 4.91368E+01 4.98845E+01 5.11967E+01 5.28993E+01 5.47641E+01 5.66347E+01 5.84254E+01 6.00946E+01 6.16245E+01 6.30087E+01 6.42465E+01 6.53396E+01 6.62905E+01 6.71016E+01 6.77751E+01 6.83123E+01 6.87145E+01 6.89822E+01 6.91828E+01
6.00657E+01 6.05488E+01 6.12345E+01 6.22988E+01 6.36573E+01 6.51848E+01 6.67723E+01 6.83431E+01 6.98482E+01 7.12585E+01 7.25569E+01 7.37338E+01 7.47840E+01 7.57049E+01 7.64951E+01 7.71540E+01 7.76813E+01 7.80769E+01 7.83407E+01 7.85385E+01
7.11453E+01 7.15973E+01 7.22057E+01 7.31069E+01 7.42463E+01 7.55454E+01 7.69267E+01 7.83263E+01 7.96968E+01 8.10045E+01 8.22266E+01 8.33478E+01 8.43578E+01 8.52500E+01 8.60198E+01 8.66645E+01 8.71821E+01 8.75712E+01 8.78310E+01 8.80262E+01
8.19235E+01 8.23388E+01 8.36769E+01 8.46755E+01 8.58238E+01 8.70627E+01 8.83388E+01 8.96080E+01 9.08361E+01 9.19973E+01 9.30729E+01 9.40494E+01 9.49173E+01 9.56698E+01 9.63022E+01 9.68112E+01 9.71947E+01 9.74511E+01 9.76439E+01
9.24248E+01 9.28120E+01 9.33148E+01 9.40410E+01 9.49550E+01 9.60116E+01 9.71615E+01 9.83582E+01 9.95605E+01 1.00735E+02 1.01854E+02 1.02897E+02 1.03850E+02 1.04700E+02 1.05440E+02 1.06063E+02 1.06566E+02 1.06945E+02 1.07199E+02 1.07390E+02
1.07790E+02 1.08155E+02 1.08626E+02 1.09305E+02 1.10161E+02 1.11153E+02 1.12240E+02 1.13379E+02 1.14531E+02 1.15665E+02 1.16751E+02 1.17770E+02 1.18704E+02 1.19540E+02 1.20270E+02 1.20886E+02 1.21383E+02 1.21759E+02 1.22011E+02 1.22201E+02
```

Fluxes in x-dir. (cm3/(cm2.t))

```
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 1.47451E-06 2.25730E-06 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 -3.70560E-05 -1.52021E-05 8.24541E-06 1.55951E-05 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 -4.83920E-04 -4.51136E-04 -2.35908E-04 -5.34728E-05 6.00699E-05 8.39712E-05 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 -2.79892E-03 -3.51338E-03 -2.57668E-03 -1.70991E-03 -7.91450E-04 -3.13624E-05 4.07453E-04 4.46524E-04 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 -1.20705E-02 -1.35435E-02 -1.24174E-02 -9.49559E-03 -5.88215E-03 -2.25690E-03 7.12411E-04 2.36707E-03 2.95008E-03 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -9.23617E-01 -3.65577E-01 -1.58098E-01 -7.61626E-02 -3.66437E-02 -1.85260E-02 -4.79259E-02 -5.62932E-02 -5.57715E-02 -4.80514E-02 -3.56929E-02 -2.10049E-02 -6.14971E-03 6.32702E-03 1.32891E-02 1.22052E-02 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -4.40796E-01 -3.34903E-01 -2.22611E-01 -1.55796E-01 -7.68262E-02 4.13460E-02 -1.89166E-01 -2.57987E-01 -2.79553E-01 -2.80989E-01 -2.69469E-01 -2.46953E-01 -2.13927E-01 -1.70834E-01 -1.19001E-01 -6.15063E-02 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -2.92916E-01 -3.04661E-01 -3.81753E-01 -6.00049E-01 -7.95587E-01 -1.11581E+00 -1.51920E+00 -1.55952E+00 -1.46176E+00 -1.30921E+00 -1.13431E+00 -9.50735E-01 -7.64453E-01 -5.77584E-01 -3.89540E-01 -1.97910E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -6.23799E-01 -1.39005E+00 -2.38524E+00 -2.96429E+00 -2.93987E+00 -2.70346E+00 -2.05292E+00 -1.76155E+00 -1.54874E+00 -1.35178E+00 -1.15762E+00 -9.64325E-01 -7.71940E-01 -5.80282E-01 -3.88655E-01 -1.94953E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -2.12658E+00 -4.89873E+00 -4.42565E+00 -3.32188E+00 -3.00293E+00 -2.66433E+00 -2.15764E+00 -1.83563E+00 -1.59142E+00 -1.37564E+00 -1.17108E+00 -9.71936E-01 -7.75995E-01 -5.81969E-01 -3.88655E-01 -1.94953E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -2.93534E+00 -4.90761E+00 -2.89116E+00 -3.41644E+00 -3.02474E+00 -2.65801E+00 -2.18516E+00 -1.85721E+00 -1.60450E+00 -1.38314E+00 -1.17535E+00 -9.74345E-01 -7.77270E-01 -5.82503E-01 -3.88720E-01 -1.94817E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -3.88287E+00 -5.02013E+00 -4.33177E+00 -3.49176E+00 -3.04554E+00 -2.65593E+00 -2.20689E+00 -1.87578E+00 -1.61634E+00 -1.39011E+00 -1.17935E+00 -9.76596E-01 -7.78453E-01 -5.82997E-01 -3.88789E-01 -1.94707E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -5.02990E+00 -5.20566E+00 -4.38048E+00 -3.55113E+00 -3.06409E+00 -2.65623E+00 -2.22389E+00 -1.89148E+00 -1.62684E+00 -1.39645E+00 -1.18303E+00 -9.78662E-01 -7.79528E-01 -5.83442E-01 -3.88853E-01 -1.94611E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -2.23351E+01 -8.67981E+00 -5.43124E+00 -4.42936E+00 -3.59723E+00 -3.07946E+00 -2.65751E+00 -2.23691E+00 -1.90448E+00 -1.40211E+00 -1.18635E+00 -9.80519E-01 -7.80481E-01 -5.83826E-01 -3.88986E-01 -1.94284E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -1.05263E+01 -8.18134E+00 -5.83837E+00 -4.55562E+00 -3.69720E+00 -3.11406E+00 -2.66120E+00 -2.26536E+00 -1.93578E+00 -1.65924E+00 -1.41693E+00 -1.19511E+00 -9.85396E-01 -7.82934E-01 -5.84771E-01 -3.89986E-01 -1.94284E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -1.11051E+01 -7.34854E+00 -5.45668E+00 -4.34173E+00 -3.58852E+00 -3.04146E+00 -2.61031E+00 -2.24651E+00 -1.93494E+00 -1.66375E+00 -1.42115E+00 -1.19759E+00 -9.86276E-01 -7.82722E-01 -5.83969E-01 -3.88042E-01 -1.93600E-01 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 -3.75652E+00 -4.65107E+00 -4.29809E+00 -3.76611E+00 -3.27368E+00 -2.85295E+00 -2.49208E+00 -2.17542E+00 -1.89372E+00 -1.63966E+00 -1.40634E+00 -1.18781E+00 -9.79400E-01 -7.77709E-01 -5.80339E-01 -3.85615E-01 -1.92354E-01 0.00000E+00
```

```
0.00000E+00 -3.23818E-01 -9.53819E-01 -2.43941E+00 -3.20115E+00 -3.31850E+00 -3.15093E+00 -2.88716E+00 -2.60458E+00 -2.32964E+00 -2.06938E+00 -1.82488E+00 -1.59482E+00 -1.37675E+00 -1.16792E+00 -9.65804E-01 -7.68374E-01 -5.74064E-01 -3.81723E-01 -1.90502E-01  0.00000E+00
0.00000E+00 -4.43515E-01 -1.05205E+00 -1.84616E+00 -2.39562E+00 -2.62381E+00 -2.63196E+00 -2.51944E+00 -2.34854E+00 -2.15251E+00 -1.94757E+00 -1.74158E+00 -1.53800E+00 -1.33793E+00 -1.14130E+00 -9.47527E-01 -7.55917E-01 -5.65822E-01 -3.76711E-01 -1.88171E-01  0.00000E+00
0.00000E+00 -4.53202E-01 -9.64694E-01 -1.49756E+00 -1.91135E+00 -2.14917E+00 -2.23367E+00 -2.21005E+00 -2.11778E+00 -1.98427E+00 -1.82681E+00 -1.65588E+00 -1.47766E+00 -1.29567E+00 -1.11182E+00 -9.27089E-01 -7.41944E-01 -5.56594E-01 -3.71129E-01 -1.85592E-01  0.00000E+00
0.00000E+00 -4.24029E-01 -8.55971E-01 -1.26802E+00 -1.60307E+00 -1.82785E+00 -1.94350E+00 -1.96931E+00 -1.92821E+00 -1.83997E+00 -1.71952E+00 -1.57747E+00 -1.42169E+00 -1.25527E+00 -1.08322E+00 -9.07065E-01 -7.28178E-01 -5.47482E-01 -3.65617E-01 -1.83050E-01  0.00000E+00
0.00000E+00 -3.89580E-01 -7.67143E-01 -1.11548E+00 -1.40507E+00 -1.61565E+00 -1.74316E+00 -1.79548E+00 -1.78580E+00 -1.72788E+00 -1.63383E+00 -1.51338E+00 -1.37396E+00 -1.22109E+00 -1.05874E+00 -8.89771E-01 -7.16219E-01 -5.39541E-01 -3.60806E-01 -1.80831E-01  0.00000E+00
0.00000E+00 -3.63144E-01 -7.07544E-01 -1.02167E+00 -1.28607E+00 -1.48654E+00 -1.61802E+00 -1.68366E+00 -1.69161E+00 -1.65192E+00 -1.57455E+00 -1.46826E+00 -1.34030E+00 -1.19638E+00 -1.04087E+00 -8.77062E-01 -7.07387E-01 -5.33656E-01 -3.57234E-01 -1.79181E-01  0.00000E+00
0.00000E+00 -3.42234E-01 -6.63557E-01 -9.55556E-01 -1.20348E+00 -1.39634E+00 -1.52906E+00 -1.60248E+00 -1.62178E+00 -1.59452E+00 -1.52899E+00 -1.43309E+00 -1.31375E+00 -1.17670E+00 -1.02653E+00 -8.66797E-01 -7.00221E-01 -5.28868E-01 -3.54322E-01 -1.77834E-01  0.00000E+00
```

        Fluxes in z-dir. (cm3/(cm2.t))
```
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  2.50000E+00  2.50000E+00  2.50000E+00  2.50000E+00  2.50000E+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  2.50000E+00  2.50000E+00  2.50004E+00  2.49998E+00  2.49999E+00  2.50002E+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  2.50000E+00  2.50000E+00  2.50048E+00  2.49997E+00  2.49982E+00  2.49980E+00  2.49986E+00  2.49997E+00  2.50010E+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  2.50000E+00  2.50280E+00  2.50427E+00  2.49971E+00  2.49910E+00  2.49890E+00  2.49904E+00  2.49942E+00  2.49993E+00  2.50055E+00
0.00000E+00  0.00000E+00  0.00000E+00  2.50000E+00  2.50000E+00  2.50000E+00  2.50000E+00  2.50000E+00  2.50000E+00  2.51207E+00  2.50427E+00  2.49943E+00  2.49793E+00  2.49549E+00  2.49607E+00  2.49777E+00  2.50000E+00  2.50284E+00
0.00000E+00  0.00000E+00  0.00000E+00  9.23614E-01  1.94196E+00  2.29252E+00  2.41806E+00  2.46048E+00  2.48188E+00  2.52940E+00  2.52044E+00  2.50375E+00  2.49170E+00  2.48443E+00  2.48080E+00  2.48042E+00  2.48359E+00  2.49081E+00  2.50109E+00  2.51505E+00
0.00000E+00  0.00000E+00  0.00000E+00  1.36441E+00  1.83606E+00  2.18023E+00  2.35125E+00  2.38151E+00  2.36371E+00  2.75991E+00  2.58925E+00  2.52531E+00  2.49314E+00  2.47290E+00  2.45828E+00  2.44739E+00  2.44049E+00  2.43897E+00  2.44359E+00  2.45354E+00
0.00000E+00  0.00000E+00  0.00000E+00  1.65732E+00  1.84780E+00  2.25732E+00  2.56954E+00  2.57704E+00  2.68393E+00  3.16329E+00  2.62958E+00  2.42755E+00  2.34058E+00  2.29801E+00  2.27470E+00  2.26111E+00  2.25362E+00  2.25092E+00  2.25196E+00  2.25563E+00
0.00000E+00  0.00000E+00  0.00000E+00  2.28112E+00  2.61405E+00  3.25250E+00  3.14859E+00  2.55262E+00  2.44752E+00  2.51274E+00  2.33820E+00  2.21474E+00  2.14361E+00  2.10384E+00  2.08140E+00  2.06872E+00  2.06196E+00  2.05915E+00  2.05890E+00  2.06017E+00
0.00000E+00  0.00000E+00  0.00000E+00  2.70643E+00  3.16848E+00  3.12407E+00  2.96164E+00  2.48882E+00  2.37979E+00  2.41140E+00  2.27379E+00  2.16589E+00  2.10044E+00  2.06292E+00  2.04157E+00  2.02952E+00  2.02315E+00  2.02048E+00  2.02016E+00  2.02118E+00
0.00000E+00  0.00000E+00  0.00000E+00  3.29350E+00  3.56292E+00  3.00036E+00  2.78709E+00  2.41047E+00  2.30643E+00  2.31682E+00  2.20819E+00  2.11533E+00  2.05616E+00  2.02135E+00  2.00135E+00  1.99010E+00  1.98418E+00  1.98171E+00  1.98137E+00  1.98220E+00
0.00000E+00  0.00000E+00  0.00000E+00  4.07007E+00  3.79036E+00  2.86267E+00  2.61908E+00  2.32122E+00  2.22850E+00  2.22700E+00  2.14196E+00  2.06343E+00  2.01090E+00  1.97919E+00  1.96079E+00  1.95046E+00  1.94508E+00  1.94286E+00  1.94254E+00  1.94326E+00
0.00000E+00  0.00000E+00  0.00000E+00  5.07605E+00  3.82550E+00  2.69762E+00  2.45324E+00  2.23376E+00  2.14692E+00  2.07546E+00  2.01050E+00  1.96481E+00  1.93649E+00  1.91991E+00  1.91062E+00  1.90586E+00  1.90394E+00  1.90369E+00  1.90432E+00
0.00000E+00  0.00000E+00  0.00000E+00  2.34500E+00  3.17578E+00  2.49724E+00  2.28681E+00  2.12020E+00  2.05639E+00  2.00897E+00  1.95679E+00  1.91803E+00  1.89333E+00  1.87874E+00  1.87061E+00  1.86652E+00  1.86495E+00  1.86481E+00  1.86541E+00
-2.73952E+00 -3.22525E+00 -7.93558E+00 -3.75652E+00 -1.05905E+00  9.95397E-02  6.75163E-01  9.89997E-01  1.17851E+00  1.29674E+00  1.36782E+00  1.40904E+00  1.43313E+00  1.44793E+00  1.45771E+00  1.46459E+00  1.46960E+00  1.47323E+00  1.47566E+00  1.47753E+00
-2.73952E+00 -3.22525E+00 -4.17907E+00 -2.86196E+00 -1.41204E+00 -4.32443E-01  1.82736E-01  5.69262E-01  8.17632E-01  9.80076E-01  1.08612E+00  1.15497E+00  1.19981E+00  1.22940E+00  1.24929E+00  1.26289E+00  1.27223E+00  1.27850E+00  1.28239E+00  1.28517E+00
-2.41570E+00 -2.59525E+00 -2.69348E+00 -2.10022E+00 -1.29469E+00 -6.00008E-01 -8.10395E-02  2.86682E-01  5.42687E-01  7.19812E-01  8.41618E-01  9.24914E-01  9.81738E-01  1.02056E+00  1.04718E+00  1.06546E+00  1.07791E+00  1.08616E+00  1.09117E+00  1.09467E+00
-1.97219E+00 -1.98672E+00 -1.89936E+00 -1.55076E+00 -1.06650E+00 -5.91859E-01 -1.93567E-01  1.15821E-01  3.46621E-01  5.14866E-01  6.35627E-01  7.21329E-01  7.81667E-01  8.23928E-01  8.53406E-01  8.73844E-01  8.87817E-01  8.97044E-01  9.02626E-01  9.06494E-01
-1.51899E+00 -1.47523E+00 -1.36650E+00 -1.13697E+00 -8.28684E-01 -5.07362E-01 -2.17191E-01  3.35468E-02  2.13109E-01  3.57406E-01  4.64695E-01  5.43106E-01  5.99675E-01  6.40077E-01  6.68674E-01  6.88698E-01  7.02464E-01  7.11576E-01  7.17088E-01  7.20901E-01
-1.09496E+00 -1.04328E+00 -9.54456E-01 -8.01913E-01 -6.03908E-01 -3.91714E-01 -1.75238E-01  2.96954E-02  1.94864E-01  3.22641E-01  4.17308E-01  4.87520E-01  5.37028E-01  5.72501E-01  5.98065E-01  6.16856E-01  6.30948E-01  6.42090E-01  6.51497E-01  6.60128E-01
-7.05377E-01 -6.65723E-01 -6.06124E-01 -5.12320E-01 -3.93323E-01 -2.64206E-01 -1.39061E-01 -2.72407E-02  6.69467E-02  1.42904E-01  2.02188E-01  2.47308E-01  2.80972E-01  3.05680E-01  3.23545E-01  3.36254E-01  3.45087E-01  3.50971E-01  3.54543E-01  3.57017E-01
-3.42233E-01 -3.21323E-01 -2.91998E-01 -2.47921E-01 -1.92858E-01 -1.32724E-01 -7.34183E-02 -1.92960E-02  2.72590E-02  6.55285E-02  9.59000E-02  1.19346E-01  1.37049E-01  1.50171E-01  1.59733E-01  1.66577E-01  1.71354E-01  1.74547E-01  1.76488E-01  1.77835E-01
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        :        1.2351356875E-02 ml/d
        Total amount that passed top layer      :        2.7563620809E+03 ml
        Total amount that passed bottom layer   :        0.0000000000E+00 ml
        Total amount that passed left boundary  :       -2.3504030914E+03 ml
        Total amount that passed right boundary :        0.0000000000E+00 ml
```

Table 15-31. Example of solute results file SNAME.

```
        TIME =   0.00000000E+00

                                        1
        Total nutrient          :        1.2078535348E+02 mmol
        Total change nutrient   :        0.0000000000E+00 mmol
        Total uptake nutrient   :        0.0000000000E+00 mmol
        Balance nutrient        :       -3.2684965845E-13 mmol
        Relative nutrient       :       -2.7060371895E-15
```

        Concentration (mmol/l) NO3
```
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 1.00000E+01 1.00000E+01 1.00000E+01
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 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
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 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
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 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 2.13109E+01 1.00000E+01 4.64905E+01 5.43106E+01 5.99675E+01 6.40077E+01 6.86574E+01 6.88698E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
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1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01 1.00000E+01
```

                                                                         1
          Total amount of N that passed top layer   :   -4.9737991503E-20 mmol
          Total amount of N that passed bottom layer   :   0.0000000000E+00 mmol
          Total amount of N that passed left boundary   :   0.0000000000E+00 mmol
          Total amount of N that passed right boundary :   0.0000000000E+00 mmol

          TIME = 1.00000000E+01

                                                                         1
          Total nutrient   :   8.7986150200E+01 mmol
          Total change nutrient :   -3.2799203275E+01 mmol
          Total uptake nutrient :   0.0000000000E+00 mmol
          Balance nutrient   :   -7.3185901783E-13 mmol
          Relative nutrient   :   -8.3178888514E-15

          Concentration (mmol/l) NO3

          Salt fluxes in x-direction (mmol/(cm2.d) NO3

          Salt fluxes in z-direction (mmol/(cm2.d) NO3

```
0.00000E+00  0.00000E+00  0.00000E+00  1.33440E-03  2.96384E-04  1.70847E-04  1.68747E-04  1.70894E-04  1.76624E-04  2.44141E-04  7.83545E-04  1.65533E-03  1.99259E-03  3.37575E-03  3.89062E-03  5.85028E-03  6.55214E-03  8.93481E-03  9.39119E-03  9.48203E-03
0.00000E+00  0.00000E+00  0.00000E+00  3.43753E-03  1.01735E-03  7.06740E-04  6.76274E-04  6.62957E-04  6.64496E-04  1.07256E-03  2.14460E-03  3.51656E-03  4.19656E-03  5.98876E-03  6.79509E-03  8.97453E-03  9.82832E-03  1.21704E-02  1.26148E-02  1.26913E-02
0.00000E+00  0.00000E+00  0.00000E+00  6.27649E-03  2.49365E-03  1.99936E-03  2.00780E-03  2.08102E-03  2.60072E-03  4.22466E-03  5.35907E-03  6.54554E-03  7.47605E-03  8.98888E-03  9.99808E-03  1.17263E-02  1.26255E-02  1.43638E-02  1.46937E-02  1.47304E-02
0.00000E+00  0.00000E+00  0.00000E+00  1.04673E-02  5.83037E-03  5.67629E-03  5.43372E-03  4.83948E-03  5.38031E-03  6.72079E-03  8.43520E-03  9.66877E-03  1.06418E-02  1.18133E-02  1.27170E-02  1.39299E-02  1.46556E-02  1.57842E-02  1.59964E-02  1.60131E-02
0.00000E+00  0.00000E+00  0.00000E+00  1.20080E-02  7.21327E-03  5.89360E-03  5.64746E-03  5.34218E-03  5.94968E-03  7.32736E-03  9.05532E-03  1.02780E-02  1.12441E-02  1.23445E-02  1.32121E-02  1.43203E-02  1.50003E-02  1.60098E-02  1.61978E-02  1.62119E-02
0.00000E+00  0.00000E+00  0.00000E+00  1.39625E-02  8.39244E-03  6.17068E-03  5.92752E-03  5.86056E-03  6.54792E-03  7.95601E-03  9.66642E-03  1.08681E-02  1.18141E-02  1.28394E-02  1.36603E-02  1.46638E-02  1.52927E-02  1.61875E-02  1.63526E-02  1.63644E-02
0.00000E+00  0.00000E+00  0.00000E+00  1.64547E-02  9.32292E-03  6.46648E-03  6.25295E-03  6.38838E-03  7.16092E-03  8.58979E-03  1.02599E-02  1.14298E-02  1.23440E-02  1.32913E-02  1.40578E-02  1.49580E-02  1.55323E-02  1.63176E-02  1.64611E-02  1.64711E-02
0.00000E+00  0.00000E+00  0.00000E+00  1.96830E-02  9.91215E-03  6.73710E-03  6.60018E-03  6.91547E-03  7.77298E-03  9.20905E-03  1.08217E-02  1.19499E-02  1.28226E-02  1.36906E-02  1.43972E-02  1.51974E-02  1.57155E-02  1.63983E-02  1.65217E-02  1.65302E-02
0.00000E+00  0.00000E+00  0.00000E+00  8.20410E-03  8.67231E-03  6.95056E-03  6.95557E-03  7.44080E-03  8.38050E-03  9.81893E-03  1.13638E-02  1.24363E-02  1.32566E-02  1.40427E-02  1.46851E-02  1.53879E-02  1.58484E-02  1.64346E-02  1.65379E-02  1.65453E-02
0.00000E+00  0.00000E+00  0.00000E+00 -8.20655E-04  3.22828E-03  5.54877E-03  7.24730E-03  8.64028E-03  9.95852E-03  1.12966E-02  1.24929E-02  1.33228E-02  1.39204E-02  1.44168E-02  1.48083E-02  1.51875E-02  1.54421E-02  1.57288E-02  1.57833E-02  1.57931E-02
-2.73950E-02 -3.22429E-02 -7.85480E-02 -3.71348E-02 -1.03935E-02  5.04211E-04  4.90884E-03  7.58584E-03  9.46453E-03  1.09012E-02  1.19785E-02  1.27118E-02  1.32155E-02  1.35852E-02  1.38568E-02  1.40819E-02  1.42346E-02  1.43780E-02  1.44175E-02  1.44353E-02
-2.73950E-02 -3.22429E-02 -7.85480E-02 -4.17873E-02 -1.40926E-02 -4.33472E-03  1.61470E-03  5.17489E-03  7.54541E-03  9.19233E-03  1.03393E-02  1.11176E-02  1.16461E-02  1.20122E-02  1.22677E-02  1.24539E-02  1.25804E-02  1.26767E-02  1.27194E-02  1.27466E-02
-2.41571E-02 -2.59525E-02 -2.69368E-02 -2.10040E-02 -1.29471E-02 -6.00152E-03 -8.20158E-04  2.79651E-03  5.30829E-03  7.06711E-03  8.29530E-03  9.14485E-03  9.73060E-03  1.01355E-02  1.04156E-02  1.06110E-02  1.07439E-02  1.08347E-02  1.08854E-02  1.09201E-02
-1.97219E-02 -1.98672E-02 -1.89938E-02 -1.55078E-02 -1.06651E-02 -5.91878E-03 -1.93647E-03  1.15262E-03  3.45116E-03  5.12859E-03  6.33574E-03  7.19446E-03  7.80044E-03  8.22589E-03  8.52325E-03  8.73001E-03  8.87131E-03  8.96517E-03  9.02102E-03  9.05960E-03
-1.51899E-02 -1.47523E-02 -1.36651E-02 -1.13697E-02 -8.28686E-03 -5.07364E-03 -2.17197E-03  2.35207E-04  2.12982E-03  3.57193E-03  4.64448E-03  5.42862E-03  5.99455E-03  6.39890E-03  6.68520E-03  6.88577E-03  7.02365E-03  7.11498E-03  7.17008E-03  7.20818E-03
-1.09496E-02 -1.04329E-02 -9.54461E-03 -8.01917E-03 -6.03911E-03 -3.91715E-03 -1.91380E-03 -1.75534E-04  1.24857E-03  2.36939E-03  3.22622E-03  3.86706E-03  4.33831E-03  4.68013E-03  4.92500E-03  5.09797E-03  5.21757E-03  5.29700E-03  5.34511E-03  5.37840E-03
-7.05377E-03 -6.65725E-03 -6.06128E-03 -5.12324E-03 -3.93326E-03 -2.64207E-03 -1.39062E-03 -2.72409E-04  6.69465E-04  1.42904E-03  2.02188E-03  2.47308E-03  2.80971E-03  3.05679E-03  3.23545E-03  3.36254E-03  3.45086E-03  3.50971E-03  3.54543E-03  3.57017E-03
-3.42233E-03 -3.21324E-03 -2.92000E-03 -2.47922E-03 -1.92859E-03 -1.32725E-03 -7.34186E-04 -1.92960E-04  2.72590E-04  6.55285E-04  9.59001E-04  1.19346E-03  1.37049E-03  1.50171E-03  1.59733E-03  1.66577E-03  1.71355E-03  1.74547E-03  1.76489E-03  1.77835E-03
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
```

1

```
Total amount of N that passed top layer     :   -1.2423346852E+01 mmol
Total amount of N that passed bottom layer  :    0.0000000000E+00 mmol
Total amount of N that passed left boundary :   -2.0375856423E+01 mmol
Total amount of N that passed right boundary :   0.0000000000E+00 mmol
```

15.6 The rerun facility

There is a special utility in the TTUTIL library (van Kraalingen and Rappoldt, 2000) 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 15.4) 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 15-32. 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. In this example the user is interested in the effect of different rain intensities for two soils, and for each run a different output file for water is used.

Table 15-32. Example of a RERUNS.DAT file.

```
* run 2
soilns = 1*'zandb3'
rain   = 365*1.0
wname  = 'zand2'
* run 3
soilns = 1*'zandb3'
rain   = 365*1.5
wname  = 'zand3'
* run 4
soilns = 1*'kleib10'
rain   = 365*0.5
wname  = 'klei1'
* run 5
soilns = 1*'kleib10'
rain   = 365*1.0
wname  = 'klei2'
* run 6
soilns = 1*'kleib10'
rain   = 365*1.5
wname  = 'klei3'
```

In this example six runs are done, three with a soil named 'zandb3' 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.

15.7 Acknowledgements

The author acknowledges Falentijn Assinck for critically reading this chapter.

15.8 References

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