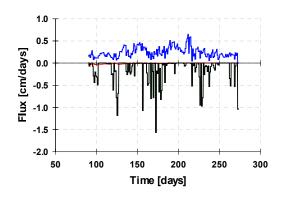
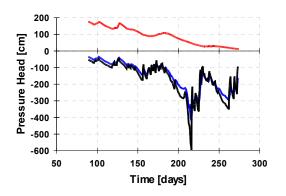
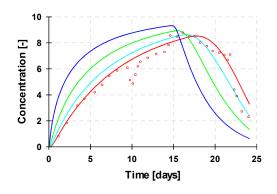
The HYDRUS-1D Software Package for Simulating the

One-Dimensional Movement of Water, Heat, and

Multiple Solutes in Variably-Saturated Media







Version 3.0

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10. PROBLEM DEFINITION

10.1. Construction of Finite Element Mesh

The finite element mesh is constructed by dividing the soil profile into linear elements whose sizes are defined by the *x*-coordinates of the nodes that form the element corners. Neighboring elements should have approximately the same size. The ratio of the sizes of two neighboring elements is not recommended to exceed about 1.5. The nodes are numbered sequentially from 1 to *NumNP* (total number of nodes) from the bottom of the soil profile to the soil surface.

The element dimensions must be adjusted to a particular problem. They should be made relatively small at locations where large hydraulic gradients are expected. Such a region is usually located close to the soil surface where highly variable meteorological factors can cause rapid changes in the soil water content and corresponding pressure heads. Therefore, it is usually recommended to use relatively small elements near the soil surface, and gradually larger sizes with depth. The element dimensions are also dependent on soil hydraulic properties. Coarse textured soils generally require a finer discretization than fine-textured soils (loams, clays). No special restrictions are necessary to facilitate the soil root zone.

10.2. Coding of Soil Types and Subregions

Soil Types - An integer code beginning with 1 and ending with NMat (the total number of soil materials) is assigned to each soil type in the flow region. The appropriate material code is subsequently assigned to each nodal point n of the finite element mesh.

Interior material interfaces do not coincide with element boundaries. When different material numbers are assigned to the nodes of a certain element, the finite element algorithm will assume that the material properties will change linearly over the element. This procedure will somewhat smooth soil interfaces. A set of soil hydraulic parameters, and solute and heat transport characteristics must be specified for each soil material.

Subregions - Water and solute mass balances are computed separately for each specified subregion. The subregions may or may not coincide with the material regions. Subregions are characterized by an integer code, which runs from 1 to NLay (the total number of subregions). A subregion code is assigned to each element in the flow domain.

10.3. Coding of Boundary Conditions

Boundary codes *KodTop* and *KodBot* must be assigned to surface and bottom boundary nodes, respectively. If a boundary node is to have a prescribed pressure head during a time step (a Dirichlet boundary condition), *KodTop* and *KodBot* must be set positive during that time step. If the volumetric flux of water entering or leaving the system is prescribed during a certain time step (a Neumann boundary condition), *KodTop* and *KodBot* must be negative or zero.

Constant Boundary Conditions - The value of a constant boundary condition for a particular boundary node, n, is given by the initial value of the pressure head, h(n), in case of Dirichlet boundary conditions, or by the initial value of the recharge/discharge flux, rTop or rBot, in case of Neumann boundary conditions. Table 10.1 summarizes the use of the variables KodTop (KodBot), rTop (rBot), and h(n) for various types of nodes.

Table 10.1. Initial settings of KodTop (KodBot), rTop (rBot), and h(n) for constant boundary conditions.

Node Type Kod7	Fop (KodBot)	rTop (rBot)	h(n)
Specified Head Boundary	1	0.0	Prescribed
Specified Flux Boundary	-1	Prescribed	Initial Value

Variable Boundary Conditions - Four types of variable boundary conditions can be imposed:

- 1. Atmospheric boundary conditions for which *TopInf=AtmInf=.true*.,
- 2. Variable pressure head boundary conditions for which *TopInf=.true*. and *KodTop=+3*, or *BotInf=.true*. and *KodBot=+3*, or
- 3. Variable flux boundary conditions for which *TopInf=.true*. and *KodTop=-3*, or *BotInf=.true*. and *KodBot=-3*.
- 4. Variable pressure head/flux boundary conditions for which *TopInf=.true*. and *KodTop=-3* or +3.

Initial settings of the variables KodTop (KodBot), rTop (rBot), and h(n) for the time-dependent boundary conditions are given in Table 10.2.

Table 10.2. Initial settings of KodTop (KodBot), rTop (rBot), and h(n) for time-variable boundary conditions.

Node Type	KodTop (KodBot)	rTop (rBot)	h(n)
Atmospheric Boundary	-4	0.0	Initial Value
Variable Head Boundary	+3	0.0	Initial Value
Variable Flux Boundary	-3	0.0	Initial Value

Atmospheric boundary conditions are implemented when *TopInf=AtmInf=.true.*, in which case time-dependent input data for the precipitation, *Prec*, and evaporation, *rSoil*, rates must be specified in the input file ATMOSPH.IN. The potential fluid flux across the soil surface is determined by *rAtm=rSoil-Prec*. The actual surface flux is calculated internally by the program. Two limiting values of surface pressure head must also be provided: *hCritS* which specifies the maximum allowed pressure head at the soil surface (usually 0.0), and *hCritA* which specifies the minimum allowed surface pressure head (defined from equilibrium conditions between soil water and atmospheric vapor). The program automatically switches the value of *KodTop* from -4 to +4 if one of these two limiting points is reached. Table 10.3 summarizes the use of the variables *rAtm*, *hCritS* and *hCritA* during program execution.

Variable head or flux boundary conditions on the soil surface (bottom of the soil profile) are implemented when $KodTop\ (KodBot)=+3$ or -3 and $TopInf\ (BotInf)=$.true., respectively. In that case, the input file ATMOSPH.IN must contain the prescribed time-dependent values of the pressure head, $hT\ (hB)$, or the flux, $rT\ (rB)$, imposed on the boundary. The values of $hT\ (hB)$ or $rT\ (rB)$ are assigned to particular nodes at specified times according to rules given in Table 10.4.

Table 10.3. Definition of the variables KodTop, rTop, and h(n) when an atmospheric boundary condition is applied.

KodTop	rTop	h(n)	Event
-4	rAtm	Unknown	rAtm=rSoil-Prec
+4	Unknown	hCritA	Evaporation capacity is exceeded
+4	Unknown	hCritS	Infiltration capacity is exceeded

Table 10.4. Definition of the variables KodTop (KodBot), rTop (rBot), and h(n) when variable head or flux boundary conditions are applied.

Node Type Ko	odTop (KodBot)	rTop (rBot)	h(n)
Variable Head Boundary	+-3	Unknown	hT(hB)
Variable Flux Boundary	-3	rT(rB)	Unknown

Water Uptake by Plant Roots - The program calculates the rate at which plants extract water from the root zone by evaluating equation (2.6). Values of the potential transpiration rate, rRoot, must be specified at preselected times in the input file ATMOSPH.IN. These time-dependent values must be provided by the user and can be calculated in various ways, such as from the temperature and crop coefficients. Actual transpiration rates are calculated internally by the program as discussed in Section 2.2. The root water uptake parameters are taken from an input file, SELECTOR.IN. Values of the function Beta(n), which describes the potential water uptake distribution over the root zone, must be specified for each node in the flow domain. If the root growth model is considered, then the exponential function for the spatial distribution of the potential root water uptake is used (equation (2.14)). All parts of the flow region where Beta(n) > 0 are treated as the soil root zone.

Root Growth Model - The program calculates the time variable rooting depth if the logical variable *lRoot* in input file SELECTOR.IN is equal to **.true**. The classical Verhulst-Pearl logistic function (2.19) (see Section 2.2) is used to model the rooting depth. The exponential

(2.14) spatial distribution function for the root water uptake function is always used along with the time-variable rooting depth option. The root growth factor, r, can be calculated either from the known value of root depth (xRMed) at a specified time (tRMed), or from the assumption that 50% of the rooting depth is reached after 50% of the growing season.

Deep Drainage from the Soil Profile - Vertical drainage, q(h), across the lower boundary of the soil profile is sometimes approximated by a flux which depends on the position of the groundwater level [e.g., Hopmans and Stricker, 1989]. If available, such a relationship can be implemented in the form of a variable flux boundary condition; the code in that case internally sets the variable KodBot equal to -7. This boundary condition will be implemented in HYDRUS if the logical variable qGWLF in the input file SELECTOR.IN is set equal to .true. The discharge rate q(n) assigned to bottom node n is determined by the program as q(n)=q(h), where h is the local value of the pressure head, and q(h) is given by

$$q(h) = -A_{ah} \exp(B_{ah} | h - GWL0L |)$$
(10.1)

where A_{qh} and B_{qh} are empirical parameters which must be specified in input file SELECTOR.IN, together with GWL0L which represents the reference position of the groundwater level (sometimes set equal to the x-coordinate of the soil surface).

Free Drainage - Unit vertical hydraulic gradient boundary conditions can be implemented in the form of a variable flux boundary condition. The program in that case will internally set the variable KodBot equal to -5. This boundary condition is implemented in HYDRUS by setting the logical variable FreeD in the input file SELECTOR. IN equal to .true. The discharge rate q(n) assigned to bottom node n is determined by the program as q(n)=-K(h), where h is the local value of the pressure head, and K(h) is the hydraulic conductivity corresponding to this pressure head.

Seepage Faces - The initial settings of the variables KodBot, rBot and h(n) for node on a seepage face are summarized in Table 10.5. This boundary condition is implemented in HYDRUS by setting the logical variable SeepF in the input file SELECTOR. IN equal to .true.

Table 10.5. Initial settings of KodBot, rBot, and h(n) for seepage faces.

Node Type	KodBot	rBot	h(n)
Seepage Face (initially saturated)	+-2	0.0	0.0
Seepage Face (initially unsaturated)	-2	0.0	Initial Value

Flow to Horizontal Drains - This boundary condition is implemented when the logical variable *lDrain* in the input file SELECTOR.IN is equal to .true. Five conceptual models can be used to describe the tile-drained soil profile:

- a) homogeneous soil profile; drain is located immediately above the impervious layer,
- b) homogeneous soil profile; drain is located some distance above the impervious layer,
- c) layered soil profile (two layers); drain is located at interface between soil layers,
- d) layered soil profile (two layers); drain is located in the bottom layer,
- e) layered soil profile (two layers); drain is located in the top layer.

The first three cases are solved with the Hooghoudt equation (2.51), and the last two cases with the Ernst equation (2.53).

Heat Transport Boundary Conditions - The type of applied boundary condition is specified by the input variables kTopT and kBotT for the upper and lower boundaries, respectively. Positive values for these variables means that a first-type boundary condition is used. When kTopT or kBotT is negative, then a third-type boundary condition is applied. On the other hand, when kBotT is equal to zero, a Neumann boundary condition with zero gradient is implemented. All initial and boundary conditions must be specified in ${}^{\circ}C$.

Solute Transport Boundary Conditions - The type of applied boundary condition is specified by the input variables kTopCh and kBotCh for the upper and lower solute transport boundaries, respectively. Similarly as for heat transport, positive values for these variables means that a first-type boundary condition will be assumed. When kTopCh or kBotCh is negative, then a third-type boundary condition is applied. When kBotCh is equal to zero, a Neumann boundary condition with zero gradient is used.

10.4. Program Memory Requirements

One single parameter statement is used at the beginning of the code to define the problem dimensions. All major arrays in the program are adjusted automatically according to these dimensions. This feature makes it possible to change the dimensions of the problem to be simulated without having to recompile all program subroutines. Different problems can be investigated by changing the dimensions in the parameter statement at the beginning of the main program, and subsequently linking all previously compiled subroutines with the main program when creating an executable file. Table 10.6 lists the array dimensions, which must be defined in the parameter statement.

Table 10.6. List of the array dimensions.

Dimension	Current setting	Description
NumNPD	1001	Maximum number of nodes in finite element mesh
NMatD	20	Maximum number of materials
NTabD	100	Maximum number of items in the table of hydraulic properties generated by the program for each soil material
NObsD	10	Maximum number of observation nodes

12. INPUT DATA

The input data for HYDRUS are given in four separate input files. These input files consist of one or more input blocks identified by the letters from A through L. The input files and blocks must be arranged as follows:

SELECTOR.IN

- A. Basic Information
- B. Water Flow Information
- C. Time Information
- D. Root Growth Information
- E. Heat Transport Information
- K. Carbon Dioxide Transport Information
- F. Solute Transport Information
- L. Major Ion Chemistry Information
- G. Root Water Uptake Information

PROFILE.DAT

H. Nodal Information

ATMOSPH.IN

I. Atmospheric Information

FIT.IN

J. Inverse Solution Information

All input files must be placed into one subdirectory. Output files are printed into the same subdirectory. Another file, **HYDRUS1D.DAT**, which is not read by the executable code, enables communication between particular modules of the user-interface and will be described in part B of this manual. The input files can be created manually or with the graphics-based user-friendly interface **HYDRUS1D** also described in part B.

Tables 12.1 through 12.12 describe the data required for each input block. All data are read in using list-directed formatting (free format). Comment lines are provided at the beginning of, and within, each input block to facilitate, among other things, proper identification of the function of the block and the input variables. The comment lines are ignored during program execution; hence, they may be left blank but should not be omitted. The program assumes that all input data are specified in a consistent set of units for mass M, length L, and time T. The values of temperature should be specified in degrees Celsius.

Most of the information in Tables 12.1 through 12.12 should be self-explanatory. Table

Table 12.1. Block A - Basic Information.

Record	Type	Variable	Description
0	Char	iVer	HYDRUS-1D version
1,2	-	-	Comment lines.
3	Char	Hed	Heading.
4	-	-	Comment line.
5	Char	LUnit	Length unit (e.g., 'cm').
6	Char	TUnit	Time unit (e.g., 'min').
7	Char	MUnit	Mass unit for concentration (e.g., 'g', 'mol', '-').
8	-	-	Comment line.
9	Logical	lWat	Set this logical variable equal to .true. when transient water flow is considered. Set this logical variable equal to .false. when initial condition is to be kept constant during the simulation.
9	Logical	lChem	Set this logical variable equal to .true. if solute transport is to be considered.
9	Logical	lTemp	Set this logical variable equal to .true. if heat transport is to be considered.
9	Logical	SinkF	Set this logical variable equal to .true. if water extraction from the root zone occurs.
9	Logical	lRoot	Set this logical variable equal to .true. if root growth is to be considered.
9	Logical	ShortF	.true. if information is to be printed only at preselected times, but not at each time step (T-level information, see Section 10), .false. if information is to be printed at each time step.
9	Logical	lWDep	.true. if hydraulic properties are to be considered as temperature dependent. .false. otherwise (see Section 2.5).
9	Logical	lScreen	.true. if information is to be printed on the screen during code execution.
9	Logical	AtmInf	.true. if variable boundary conditions are supplied via the input file ATMOSPH.IN,.false. if the file ATMOSPH.IN is not provided (i.e., in case of time independent boundary conditions).
9	Logical	lEquil [*]	.true. if equilibrium or no adsorption is considered in the solute transport equation..false. if nonequilibrium adsorption is considered for at least one solute species.
9	Logical	lInverse ⁺	.true. if inverse problem is to be solvedfalse. if direct problem is to be solved.
10	-	-	Comment line.
11	Logical	lSnow	Set this logical variable equal to .true. if snow accumulation of the soil surface is to be considered (heat transport needs to be considered as well).

Table 12.1. (continued)

Record	Type	Variable	Description
12	-	-	Comment line.
13	Integer	NMat	Number of soil materials. Materials are identified by the material number, <i>MatNum</i> , specified in Block H.
13	Integer	NLay	Number of subregions for which separate water balances are being computed. Subregions are identified by the subregion number, <i>LayNum</i> , specified in Block H.
13	Real	CosAlfa	Cosine of the angle between the flow direction and the vertical axis (i.e., $\cos \alpha = 1$ for vertical flow, $\cos \alpha = 0$ for horizontal flow, and $0 < \cos \alpha < 1$ for inclined flow.

^{*}Parameter *lEquil* is replaced with parameter *lCO2* when the major ion chemistry module is used, indicating whether or not the carbon dioxide transport is to be considered.

⁺Parameter *lInverse* is replaced with parameter *lKRed* when major ion chemistry module is used, indicating that a reduction in the hydraulic conductivity due to solution composition is to be considered.

Table 12.2. Block B - Water Flow Information.

Record	Туре	Variable	Description			
1,2	-	-	Comment lines.			
3	Integer	MaxIt	Maximum number of iterations allowed during any time step (usually 20).			
3	Real	TolTh	Absolute water content tolerance for nodes in the unsaturated part of the fregion [-] (its recommended value is 0.0001). <i>TolTh</i> represents the maxim desired absolute change in the value of the water content, θ , between a successive iterations during a particular time step.			
3	Real	TolH	Absolute pressure head tolerance for nodes in the saturated part of the flow region [L] (its recommended value is 0.1 cm). $TolH$ represents the maximum desired absolute change in the value of the pressure head, h , between two successive iterations during a particular time step.			
4	-	-	Comment line.			
5	Logical	TopInf	.true. if time dependent boundary condition is to be imposed at the top of the profile; data are supplied via input file ATMOSPH.INfalse. in the case of time independent surface boundary conditions.			
5	Logical	WLayer	Set this variable equal to .true. if water can accumulate at the surface with zero surface runoff.			
5	Integer	KodTop	Code specifying type of boundary condition (BC) for water flow at the surface. Code number is positive for Dirichlet BC and negative for Neumann BC. In the case of 'Atmospheric BC' set <i>KodTop</i> =-1. Set <i>KodTop</i> =0 when a prescribed BC can change from Dirichlet BC to Neumann BC and vice versa.			
5	Logical	lInitW	Set this variable equal to .true. if the initial condition is given in terms of the water content. Set this variable equal to .false. if the initial condition is given in terms of the pressure head			
6	-	-	Comment line.			
7	Logical	BotInf	.true. if time dependent boundary condition is to be imposed at the bottom of the profile; control data are supplied via input file ATMOSPH.IN. .false. in the case of time independent bottom boundary conditions.			
7	Logical	qGWLF	Set this variable equal to .true. if the discharge-groundwater level relationship $q(GWL)$ is applied as bottom boundary condition.			
7	Logical	FreeD	.true. if free drainage is to be considered as bottom boundary condition.			
7	Logical	SeepF	.true. if seepage face is to be considered as the bottom boundary condition.			
7	Integer	KodBot	Code specifying type of boundary condition for water flow at the bottom of the profile. Code number is positive for a Dirichlet BC and negative for a Neumann BC. In case of a seepage face or free drainage BC set <i>KodBot</i> =-1.			
7	Logical	qDrain	.true. if flow to horizontal drains is considered as bottom boundary condition.			
8a	-	-	Comment line.			

Table 12.2. (continued)

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9bReal $GWLOL$ Reference position of the groundwater table (e.g., the x-coordinate of the surface).9bReal Aqh Value of the parameter A_{qh} [LT ⁻¹] in the $q(GWL)$ -relationship, equation (10 set to zero if $qGWLF$ =.false.9bReal Bqh Value of the parameter B_{qh} [LT ⁻¹] in the $q(GWL)$ -relationship, equation (10.1) to zero if $qGWLF$ =.false.8cComment line.9cInteger $iPosDr$ Code for position of the drain. = 1: Homogeneous profile; drain on top of impervious layer. = 2: Homogeneous profile; drain above impervious layer. = 3: Layered profile; drain in bottom layer. = 5: Layered profile; drain in bottom layer. = 5: Layered profile; drain in top layer.10cComment line.11cReal $zBotDr$ Coordinate of the bottom of the drain system [L].11cReal $zBotDr$ Coordinate of the bottom of the drain system [L].11cReal $zBotDr$ Entrance resistance, $z coordinate$ (T].12cComment line.12cComment line.13cReal $z coordinate$ (T) $z coordinate$ (T)13cReal $z coordinate$ (T)13cReal $z c$				Records 8a and 9a are provided only when lower or upper boundary conditions are independent of time and at least one of them is a Neumann BC.
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set to zero if $qGWLF$ =.false. Poblished Real Bah Walue of the parameter B_{qh} [L ⁻¹] in the $q(GWL)$ -relationship, equation (10.1) to zero if $qGWLF$ =.false. Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 8b and 9b are provided only when the logical variable $qGWLF$ =.true Records 4b and 9b are provided only when the logical variable $qGWLF$ =.true Records 4b and 9b are provided only when the logical variable $qGWLF$ =.true Records 4b and 9b are provided only when the logical variable $qGWLF$ =.true Records 4b and 9b are provided only when the logical variable $qGWLF$ =.true Records 4b and 9b are provided o	9b	Real	GWL0L	Reference position of the groundwater table (e.g., the <i>x</i> -coordinate of the soil surface).
to zero if $qGWLF$ =.false. Records 8b and 9b are provided only when the logical variable $qGWLF$ =.tru 8c Comment line. 9c Integer $iPosDr$ Code for position of the drain. = 1: Homogeneous profile; drain on top of impervious layer. = 2: Homogeneous profile; drain above impervious layer. = 3: Layered profile; drain in bottom layer. = 5: Layered profile; drain in top layer. 10c Comment line. 11c Real $zBotDr$ Coordinate of the bottom of the drain system [L]. 11c Real $rSpacing$ Drain spacing, L_{dr} [L]. 11c Real $Entres$ Entrance resistance, γ_{Entr} [T]. 12c - Comment line. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT $^{-1}$]. 13c Real $BaseGW$ Coordinate of the impervious layer [L].	9b	Real	Aqh	Value of the parameter A_{qh} [LT ⁻¹] in the $q(GWL)$ -relationship, equation (10.1); set to zero if $qGWLF$ =.false.
8c - Comment line. 9c Integer $iPosDr$ Code for position of the drain. = 1: Homogeneous profile; drain on top of impervious layer. = 2: Homogeneous profile; drain above impervious layer. = 3: Layered profile; drain at interface between both soil layers. = 4: Layered profile; drain in bottom layer. = 5: Layered profile; drain in top layer. 10c - Comment line. 11c Real $zBotDr$ Coordinate of the bottom of the drain system [L]. 11c Real $rSpacing$ Drain spacing, L_{dr} [L]. 11c Real $Entres$ Entrance resistance, γ_{entr} [T]. 12c - Comment line. The following value is specified when $iPosDr = 1$. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT $^{-1}$]. The following three values are specified when $iPosDr = 2$. 13c Real $BaseGW$ Coordinate of the impervious layer [L]. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT $^{-1}$].	9b	Real	Bqh	Value of the parameter B_{qh} [L ⁻¹] in the $q(GWL)$ -relationship, equation (10.1); set to zero if $qGWLF$ =. false.
9c Integer $iPosDr$ Code for position of the drain. = 1: Homogeneous profile; drain on top of impervious layer. = 2: Homogeneous profile; drain above impervious layer. = 3: Layered profile; drain in bottom layer. = 4: Layered profile; drain in top layer. = 5: Layered profile; drain in top layer. 10c Comment line. 11c Real $zBotDr$ Coordinate of the bottom of the drain system [L]. 11c Real $rSpacing$ Drain spacing, L_{dr} [L]. 11c Real $Entres$ Entrance resistance, γ_{entr} [T]. 12c - Comment line. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹]. 13c Real $BaseGW$ Coordinate of the impervious layer [L].				Records 8b and 9b are provided only when the logical variable <i>qGWLF</i> =.true.
$= 1: \text{Homogeneous profile; drain on top of impervious layer.} \\ = 2: \text{Homogeneous profile; drain above impervious layer.} \\ = 3: \text{Layered profile; drain at interface between both soil layers.} \\ = 4: \text{Layered profile; drain in bottom layer.} \\ = 5: \text{Layered profile; drain in top layer.} \\ \\ 10c - \text{Comment line.} \\ \\ 11c \text{Real} zBotDr \text{Coordinate of the bottom of the drain system [L].} \\ \\ 11c \text{Real} rSpacing \text{Drain spacing, L_{dr} [L].} \\ \\ 11c \text{Real} Entres \text{Entrance resistance, γ_{entr} [T].} \\ \\ 12c - \text{Comment line.} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} BaseGW \text{Coordinate of the impervious layer [L].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} KhTop \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} \text{Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT^{-1}].} \\ \\ 13c \text{Real} Horizontal saturate$	8c	-	-	Comment line.
11c Real $zBotDr$ Coordinate of the bottom of the drain system [L]. 11c Real $rSpacing$ Drain spacing, L_{dr} [L]. 11c Real $Entres$ Entrance resistance, γ_{entr} [T]. 12c - Comment line. The following value is specified when $iPosDr = 1$. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹]. The following three values are specified when $iPosDr = 2$. 13c Real $BaseGW$ Coordinate of the impervious layer [L]. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].	9c	Integer	iPosDr	 = 1: Homogeneous profile; drain on top of impervious layer. = 2: Homogeneous profile; drain above impervious layer. = 3: Layered profile; drain at interface between both soil layers. = 4: Layered profile; drain in bottom layer.
11cReal $rSpacing$ Drain spacing, L_{dr} [L].11cReal $Entres$ Entrance resistance, γ_{entr} [T].12cComment line.13cReal $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT $^{-1}$].13cReal $BaseGW$ Coordinate of the impervious layer [L].13cReal $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT $^{-1}$].	10c	-	-	Comment line.
12c - Comment line. The following value is specified when $iPosDr = 1$. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹]. The following three values are specified when $iPosDr = 2$. 13c Real $BaseGW$ Coordinate of the impervious layer [L]. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].	11c	Real	rSpacing	Drain spacing, L_{dr} [L].
13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹]. The following three values are specified when $iPosDr = 2$. 13c Real $BaseGW$ Coordinate of the impervious layer [L]. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].	12c	-	-	
The following three values are specified when $iPosDr = 2$. 13c Real $BaseGW$ Coordinate of the impervious layer [L]. 13c Real $KhTop$ Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].				The following value is specified when $iPosDr = 1$.
13c Real <i>BaseGW</i> Coordinate of the impervious layer [L]. 13c Real <i>KhTop</i> Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].	13c	Real	KhTop	Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].
13c Real <i>KhTop</i> Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].				The following three values are specified when $iPosDr = 2$.
	13c	Real	BaseGW	Coordinate of the impervious layer [L].
13c Real $WetPer$ Wet perimeter of the drain, u [L].	13c	Real	KhTop	Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].
	13c	Real	WetPer	Wet perimeter of the drain, u [L].

Table 12.2. (continued)

Record	Type	Variable	Description
			The following four values are specified when $iPosDr = 3$.
13c	Real	BaseGW	Coordinate of the impervious layer [L].
13c	Real	KhTop	Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].
13c	Real	KhBot	Horizontal saturated hydraulic conductivity below the drain, K_{hBot} [LT ⁻¹].
13c	Real	WetPer	The wet perimeter, u , of the drain [L].
			The following six values are specified when $iPosDr = 4$.
13c	Real	BaseGW	Coordinate of the impervious layer [L].
13c	Real	KvTop	Vertical saturated hydraulic conductivity above the drain, K_{vTop} [LT ⁻¹].
13c	Real	KvBot	Vertical saturated hydraulic conductivity below the drain, K_{vBot} [LT ⁻¹].
13c	Real	KhBot	Horizontal saturated hydraulic conductivity below the drain, K_{hBot} [LT ⁻¹].
13c	Real	WetPer	The wet perimeter, u , of the drain [L].
13c	Real	zInTF	Coordinate of the transition between the upper and lower soil layer [L].
			The following seven values are specified when $iPosDr = 5$.
13c	Real	BaseGW	Coordinate of the impervious layer [L].
13c	Real	KhTop	Horizontal saturated hydraulic conductivity above the drain, K_{hTop} [LT ⁻¹].
13c	Real	KvTop	Vertical saturated hydraulic conductivity above the drain, K_{vTop} [LT ⁻¹].
13c	Real	KhBot	Horizontal saturated hydraulic conductivity below the drain, K_{hBot} [LT ⁻¹].
13c	Real	WetPer	The wet perimeter, u , of the drain [L].
13c	Real	zInTF	Coordinate of the transition between the upper and lower soil layers [L].
13c	Real	GeoFac	Geometry factor, a_{dr} [-], as obtained by the relaxation method [<i>Ernst</i> , 1962] (see Table below).

V / V			D_{bot}/D_t	op		
K_{hbot}/K_{htop}	1 2	4	8	16	32	
1	2.0	3.0	5.0	9.0	15.0	30.0
2	2.4	3.2	4.6	6.2	8.0	10.0
3	2.6	3.3	4.5	5.5	6.8	8.0
5	2.8	3.5	4.4	4.8	5.6	6.2
10	3.2	3.6	4.2	4.5	4.8	5.0
20	3.6	3.7	4.0	4.2	4.4	4.6
50	3.8	4.0	4.0	4.0	4.2	4.6

Table 12.2. (continued)

Record	Туре	Variable	Description
10	-	-	Comment line.
11	Real	ha	Absolute value of the upper limit [L] of the pressure head interval below which a table of hydraulic properties will be generated internally for each material (h_a must be greater than 0.0; e.g. 0.001 cm) (see Section 5.4.7).
11	Real	hb	Absolute value of the lower limit [L] of the pressure head interval for which a table of hydraulic properties will be generated internally for each material (e.g. 1000 m). One may assign to h_b the highest (absolute) expected pressure head to be expected during a simulation. If the absolute value of the pressure head during program execution lies outside of the interval $[h_a, h_b]$, then appropriate values for the hydraulic properties are computed directly from the hydraulic functions (i.e., without interpolation in the table).
12	-	-	Comment line.
13	Integer	iModel	Soil hydraulic properties model: = 0; van Genuchten's [1980] model with six parameters. = 1; modified van Genuchten's model with ten parameters [Vogel and Cislerová, 1988]. = 2; Brooks and Corey's [1964] model with six parameters. = 3; van Genuchten's [1980] model with air-entry value of -2 cm and with six parameters. = 4; Kosugi's [1996] model with six parameters. = 5; dual porosity model of Durner [1994] with nine parameters. = 6; dual-porosity system with transfer proportional to the effective saturation (9 parameters) (see Sections 2.2.1. and 2.8.). = 6; dual-porosity system with transfer proportional to the pressure head (11 parameters) (see Sections 2.2.1. and 2.8.).
			iModel>3 options are not available with the major ion chemistry module.
13	Integer	iHyst	Hysteresis in the soil hydraulic properties: = 0; No hysteresis = 1; Hysteresis in the retention curve only = 2; Hysteresis in both the retention and hydraulic conductivity functions = 3; Hysteresis using Bob Lenhard's model [Lenhard et al., 1991; Lenhard and Parker, 1992]. (Not available with major ion chemistry module.)
14	-	-	Comment line.
15	Integer	iКарра	 = -1 if the initial condition is to be calculated from the main drying branch. = 1 if the initial condition is to be calculated from the main wetting branch.
			Records 14 and 15 are provided only when $iHyst > 0$.
16	-	-	Comment line.
17 17 17	Real Real Real	Par(1,M) Par(2,M) Par(3,M)	Parameter θ_r for material M [-]. Parameter θ_s for material M [-]. Parameter α for material M [L ⁻¹].

Table 12.2. (continued)

Record	Туре	Variable	Description
17	Real	<i>Par</i> (4, <i>M</i>)	Parameter n for material $M[-]$.
17	Real	Par(5,M)	Parameter K_s for material M [LT ⁻¹].
17	Real	Par(6,M)	Parameter l for material M [-].
			The following four parameters are specified only when <i>iModel</i> =1.
17	Real	Par(7,M)	Parameter θ_m for material $M[-]$.
17	Real	Par(8,M)	Parameter θ_a for material M [-].
17	Real	Par(9,M)	Parameter θ_k for material M [-].
17	Real	Par(10,M)	Parameter K_k for material M [LT ⁻¹].
			The following four parameters are specified only when <i>iModel</i> =0 and <i>iHyst</i> >1.
17	Real	Par(7,M)	Parameter θ_m for material $M[-]$.
17	Real	Par(8,M)	Parameter θ_s^w for material $M[-]$.
17	Real	Par(9,M)	Parameter α^{w} for material $M[L^{-1}]$.
17	Real	Par(10,M)	Parameter K_s^{w} for material M [LT ⁻¹].
			The following three parameters are specified only when iModel=5 [Durner,
1994].			
17	Real	<i>Par</i> (7, <i>M</i>)	Parameter w for material M [-]. The weighting factor for the sub-curve for the second overlapping subregion.
17	Real	Par(8,M)	Parameter α for material $M[L^{-1}]$ for the second overlapping subregion.
17	Real	Par(9,M)	Parameter n for material M [-] for the second overlapping subregion.
			The following four parameters are specified only when <i>iModel</i> =6 (dual-porosity system with transfer proportional to the water content gradient).
17	Real	Par(7,M)	Parameter θ_r^{im} for the immobile region of material $M[-]$.
17	Real	Par(8,M)	Parameter θ_s^{im} for the immobile region of material M [-].
17	Real	Par(9,M)	Parameter ω (mass transfer coefficient in (2.63)) for material M [-].
			The following four parameters are specified only when <i>iModel</i> =7 (dual-porosity system with transfer proportional to the pressure head gradient).
17	Real	Par(7,M)	Parameter θ_r^{im} for the immobile region of material $M[-]$.
17	Real	Par(8,M)	Parameter θ_s^{im} for the immobile region of material $M[-]$.
17	Real	Par(9,M)	Parameter α^{im} for the immobile region of material M [-].
17	Real	Par(10,M)	Parameter n^{im} for the immobile region of material M [-].
17	Real	<i>Par</i> (11, <i>M</i>)	Parameter K_a (mass transfer coefficient in (2.67)) for material M [-].
			Record 17 information is provided for each material M (from 1 to NMat).
			If $lWDep$ =.true. (Block A) then the soil hydraulic parameters $Par(i,M)$ must be specified at reference temperature T_{ref} =20°C.

Table 12.3. Block C - Time information.

Record	Type	Variable	Description
1,2	-	-	Comment lines.
3	Real	dt	Initial time increment, Δt [T]. Initial time step should be estimated in dependence on the problem being solved. For problems with high-pressure gradients (e.g. infiltration into an initially dry soil), Δt should be relatively small.
3	Real	dtMin	Minimum permitted time increment, Δt_{min} [T].
3	Real	dtMax	Maximum permitted time increment, Δt_{max} [T].
3	Real	dMul	If the number of required iterations at a particular time step is less than or equal to $ItMin$, then Δt for the next time step is multiplied by a dimensionless number $dMul \ge 1.0$ (its value is recommended not to exceed 1.3).
3	Real	dMul2	If the number of required iterations at a particular time step is greater than or equal to $ItMax$, then Δt for the next time step is multiplied by $dMul2 \le 1.0$ (e.g. 0.33).
3	Integer	ItMin	If the number of required iterations at a particular time step is less than or equal to $ItMin$, then Δt for the next time step is multiplied by a dimensionless number $dMul \ge 1.0$ (its value is recommended not to exceed 1.3).
3	Integer	ItMax	If the number of required iterations at a particular time step is greater than or equal to $ItMax$, then Δt for the next time step is multiplied by $dMul2 \le 1.0$ (e.g. 0.33).
3	Integer	MPL	Number of specified print-times at which detailed information about the pressure head, water content, flux, temperature, concentrations, and the water and solute balances will be printed.
4	-	-	Comment line.
5	Real	tInit	Initial time of the simulation [T].
5	Real	tMax	Final time of the simulation [T].
6	-	-	Comment line.
7	Logical	lPrint	Set this logical variable equal to .true. if information about the pressure heads, water contents, temperatures, and concentrations in observation nodes, and the water and solute fluxes is to be printed at a constant time interval <i>tPrintInterval</i> .
7	Integer	nPrintSteps	Information to the screen and output files is not printed at each time step, but after each <i>nPrintSteps</i> .
7	Real	tPrintInterval	A constant time interval after which information about the pressure heads, water contents, temperatures, and concentrations in observation nodes, and the water and solute fluxes is to be printed.

Table 12.3. (continued)

Record	Type	Variable	Description
7	Logical	lEnter	Set this logical variable equal to .true. if the Enter key is to be pressed at the end of simulation.
8	-	-	Comment line.
9	Real	TPrint(1)	First specified print-time [T].
9	Real	TPrint(2)	Second specified print-time [T].
•			
9	Real	TPrint(MPL)	Last specified print-time [T]. (Maximum six values on one line.)

Table 12.4. Block D - Root Growth Information.⁺

Record	Type	Symbol	Description
1,2	-	-	Comment lines.
3	Integer	iRFak	Method to calculate the root growth factor, r .
			= 0; the root growth factor is calculated from given data [xRMed, tRMed].
			= 1; the root growth factor is calculated based on the assumption that 50% of the rooting depth, $(xRMax+xRMin)/2$., is reached at the midpoint of the growing season, $(tRMin+tRHarv)/2$.
3	Real	tRMin	Initial time of the root growth period [T].
3	Real	tRMed	Time of known rooting depth (set equal to zero if <i>iRFak</i> =1) [T].
3	Real	tRHarv	Time at the end of the root water uptake period [T].
3	Real	xRMin	Initial value of the rooting depth at the beginning of the growth period (recommended value = 1 cm) [L].
3	Real	xRMed	Value of known rooting depth (set equal to zero if <i>iRFak</i> =1) [L].
3	Real	xRMax	Maximum rooting depth, which may be reached at infinite time [L].

⁺ Block D is not needed if the logical variable *lRoot* (Block A) is set equal to **.false.**

Table 12.8. Block H - Nodal information.

Record	Type	Variable	Description
1	Integer	NFix	Number of fixed nodes.
2	Integer	i	Fixed node.
2	Real	xFix(i)	x-coordinate of the fixed node i .
2	Real	wTop(i)	Nodal density above fixed node <i>i</i> .
2	Real	wBot(i)	Nodal density below fixed node i.
			Record 2 must be specified for each fixed node.
			Records 1 and 2 have relevant information only for the module PROFILE of the user interface. When the code is used without the user interface, then only two fixed points (top and bottom of the soil profile) with unit nodal density have to be specified.
3	Integer	NumNP	Number of nodal points.
3	Integer	NS	Number of solutes (set equal to zero if <i>lChem</i> is equal to .false.).
3	Integer	iTemp	This variable is read only if the user interface is used. = 1; initial condition for the temperature is specified (must be equal to 1 when lTemp or lChem is equal to .true.). = 0; initial condition for the temperature is not specified.
3	Integer	iEquil	This variable is read only if the user interface is used. = 1; Equilibrium solute transport is considered. = 0; Nonequilibrium solute transport is considered.
			Set equal to 1 if <i>lChem</i> is equal to .false. .
4	Integer	n	Nodal number.
4	Real	x(n)	x-coordinate of node n [L].
4	Real	hNew(n)	Initial value of the pressure head at node n [L]. If $lWat=.$ false. in Block A, then $hNew(n)$ represents the pressure head which will be kept constant during simulation.
4	Integer	MatNum(n)	Index for material whose hydraulic and transport properties are assigned to node n .
4	Integer	LayNum(n)	Subregion number assigned to node <i>n</i> .
4	Real	Beta(n)	Value of the water uptake distribution, $b(x)$ [L ⁻¹], in the soil root zone at node n . Set $Beta(n)$ equal to zero if node n lies outside the root zone.
			Following three numbers, i.e., $Ah(n)$, $Ak(n)$, and $Ath(n)$, are given only when neither carbon dioxide transport nor major ion chemistry is considered.
4	Real	Ah(n)	Nodal value of the dimensionless scaling factor α_h [-] associated with the pressure head.

Table 12.8. (continued)

Record	Type	Variable	Description
4	Real	Ak(n)	Nodal value of the dimensionless scaling factor α_K [-] associated with the saturated hydraulic conductivity.
4	Real	Ath(n)	Nodal value of the dimensionless scaling factor α_{θ} [-] associated with the water content.
			The following number, i.e., $CO2(n)$, is given only when either carbon dioxide transport or major ion chemistry is considered.
4	Real	CO2(n)	Initial value of the carbon dioxide concentration at node n [L ³ L ⁻³].
4	Real	Temp(n)	Initial value of the temperature at node n [°C] (do not specify if both $lTemp$ or $lChem$ are equal to .false. ; if $lTemp$ =. false. and $lChem$ =. true. then set equal to 0 or any other initial value to be used later for temperature dependent water flow and solute transport).
			Following dissolved and sorbed concentrations, i.e., $Conc(i,n)$ and $Sorb(i,n)$, are given only when neither carbon dioxide transport nor major ion chemistry is considered.
4	Real	Conc(1,n)	Initial value of the concentration of the first solute at node n [ML ⁻³] (omit if $lChem$ =.false.).
4	Real	Conc(2,n)	Initial value of the concentration of the second solute at node n [ML ⁻³] (omit if $lChem$ =.true. and $NS < 2$).
•			•
4	Real	Conc(i,n)	Initial value of the concentration of the last solute at node n [ML ⁻³] (omit if $lChem$ =.true. and $NS < i$).
4	Real	Sorb(1,n)	Initial value of the adsorbed concentration on type-2 sites of the first solute at node n [ML ⁻³]. Omit this variable if $lChem$ =.false. or $lEquil$ =.true.
4	Real	Sorb(2,n)	Initial value of the adsorbed concentration on type-2 sites of the second solute at node n [ML ⁻³]. Omit this variable if $lChem$ =.false. or $lEquil$ =.true. or $NS < 2$.
4	Real	Sorb(i,n)	Initial value of the adsorbed concentration on type-2 sites of the <i>NS</i> th solute at node n [ML ⁻³]. This variable does not have to be specified if $lChem$ =.false. or $lEquil$ =.true. and $NS < i$).
			Following three numbers, i.e., $nC(n)$, $nX(n)$, and $nS(n)$, are given only when major ion chemistry is considered.
4	Integer	nC(n)	Code which specifies which solution concentration combination (see Block H) is to be used as an initial condition at node n [-] (omit if $lChem$ =.false.).
4	Integer	nX(n)	Code which specifies which surface species combination (see Block H) is to be used as an initial condition at node n [-] (omit if $lChem$ =.false.).
4	Integer	nS(n)	Code which specifies which mineral phase combination (see Block H) is to be used as an initial condition at node n [-] (omit if $lChem$ =.false.).

Table 12.8. (continued)

Record	Type	Variable	Description
			In general, record 4 information is required for each node n , starting with $n=1$ and continuing sequentially until $n=NumNP$. Record 4 information for certain nodes may be skipped if several conditions are satisfied (see beginning of this section).
5	Integer	NObs	Number of observation nodes for which values of the pressure head, the water content, temperature (for <i>lTemp=.true.</i>), and the solution and sorbed concentrations (for <i>lChem=.true.</i>) are printed at each time level.
6	Integer	iObs(1)	Nodal number of the first observation node.
6	Integer	iObs(2)	Nodal number of the second observation node.
6	Integer	iObs(NObs)	Nodal number of the last observation node.

Table 12.9. Block I - Atmospheric information.⁺

Record	Туре	Variable	Description
1,2	-	-	Comment lines.
3	Integer	MaxAl	Number of atmospheric data records.
4	-	-	Comment line.
5	Real	hCritS	Maximum allowed pressure head at the soil surface [L].
6	-	-	Comment line.
7	Real	tAtm(i)	Time for which the <i>i</i> -th data record is provided [T].
7	Real	Prec(i)	Precipitation rate [LT ⁻¹] (in absolute value).
7	Real	rSoil(i)	Potential evaporation rate [LT ⁻¹] (in absolute value). <i>rSoil(i)</i> is interpreted as <i>KodTop</i> when a time variable Dirichlet or Neumann boundary condition is specified.
7	Real	rRoot(i)	Potential transpiration rate [LT ⁻¹] (in absolute value).
7	Real	hCritA(i)	Absolute value of the minimum allowed pressure head at the soil surface [L].
7	Real	rB(i)	Bottom flux [LT ⁻¹] (set equal to 0 if $KodBot$ is positive, or if one of the logical variables $qGWLF$, $FreeD$ or $SeepF$ is .true.).
7	Real	hB(i)	Groundwater level [L], or any other prescribed pressure head boundary condition as indicated by a positive value of <i>KodBot</i> (set equal to 0 if <i>KodBot</i> is negative, or if one of the logical variables <i>qGWLF</i> , <i>FreeD</i> or <i>SeepF</i> is .true.).
7	Real	hT(i)	Prescribed pressure head [L] at the surface (set equal to 0 if <i>KodBot</i> is negative).
7	Real	tTop(i)	Soil surface temperature [°C] (omit if both <i>lTemp</i> and <i>lChem</i> are equal to .false.).
7	Real	tBot(i)	Soil temperature at the bottom of the soil profile [°C] (omit if both <i>lTemp</i> and <i>lChem</i> are equal to .false. , set equal to zero if <i>kBotT</i> =0).
7	Real	Ampl(i)	Temperature amplitude at the soil surface [K] (omit if both <i>lTemp</i> and <i>lChem</i> are equal to .false.).
			The following values, i.e., $cTop(i,j)$ and $cBot(i,j)$, are given only when neither carbon dioxide transport nor major ion chemistry is considered.
7	Real	cTop(i,1)	Soil surface concentration [ML ³] for the first solute (not needed if <i>lChem</i> is equal to .false.).
7	Real	cTop(i,2)	Soil surface concentration [ML ⁻³] for the second solute (not needed if <i>lChem</i> is equal to .false. or $NS < 2$).
	•	•	•
7	Real	cTop(i,NS)	Soil surface concentration [ML ⁻³] for the <i>NS</i> th solute (not needed if <i>lChem</i> is equal to .false.).
7	Real	cBot(i,1)	Concentration at the bottom of the soil profile [ML ⁻³] for the first solute (not needed if <i>lChem</i> is equal to .false. , set equal to zero if <i>cBotSolute</i> =0).

Table 12.9. (continued)

Record	Туре	Variable	Description
7	Real	cBot(i,2)	Concentration at the bottom of the soil profile [ML ⁻³] for the second solute (not needed if <i>lChem</i> is equal to .false. , set equal to zero if <i>cBotSolute</i> =0 or $NS < 2$).
7	Real	cBot(i,NS)	Concentration at the bottom of the soil profile [ML ⁻³] for the <i>NS</i> th solute (not needed if <i>lChem</i> is equal to .false. , set equal to zero if <i>cBotSolute</i> =0).
			Following two number, i.e., $kTopCh(i)$ and $kBotCh(i)$, are given only when major ion chemistry is considered.
7	Real	kTopCh(i)	Code which refers to the field $ConcTab$ for the value of the solute transport upper boundary condition. Sign of $kTopCh(i)$ indicates whether a Dirichlet (positive) or Neumann (negative) boundary condition is to be applied at the soil surface. $ConcTab(abs(kTopCh(i)),j)$ is the boundary condition for the soil surface for species j . Permissible values are $\pm 1, \pm 2, \pm 3,, \pm nSolConc$.
7	Real	kBotCh(i)	Code which refers to the field $ConcTab$ for the value of the solute transport lower boundary condition. Sign of $kBotCh(i)$ indicates whether a Dirichlet (positive) or Neumann (negative) boundary condition is to be applied at the bottom of the soil profile. $ConcTab(abs(kBotCh(i)),j)$ is the boundary condition for the bottom of the soil profile for species j . Permissible values are $\pm 1, \pm 2, \pm 3,, \pm nSolConc$.
			The total number of atmospheric data records is <i>MaxAl</i> (i=1,2,, <i>MaxAl</i>).

⁺ Block I is not needed if the logical variable *AtmInf* (Block A) is set equal to **.false.** .

13. OUTPUT DATA

The program output consists of $9+(n_s-1)$ output files (when major ion chemistry is not considered), where n_s is the number of solutes considered in the first-order decay chain. When major ion chemistry is considered the program output consists of 13 output files. The output is organized into 3 groups:

T-level information

T_LEVEL.OUT RUN_INF.OUT SOLUTE.OUT OBS_NODE.OUT CO2_INF.OUT*

P-level information

NOD_INF.OUT BALANCE.OUT CONC.OUT* SOLID.OUT* EQUIL.OUT* CHEMBAL.OUT*

A-level information A LEVEL.OUT

In addition, some of the input data are printed to files I_CHECK.OUT and PROFILE.OUT. A separate output file SOLUTE.OUT is created for each solute. Results of the inverse solution are directed into an output file FIT.OUT. All output files are directed to the same directory as the input files, which must be created by the user prior to program execution (the directory is created automatically if the user interface is used). The various output files are described in detail in this section.

File I_CHECK.OUT contains a complete description of the space discretization, the hydraulic characteristic, and the transport properties of each soil material.

^{*}Major ion chemistry module output files

Table 13.1. T_LEVEL.OUT - pressure heads and fluxes on the boundaries and in the root zone.

Time	Time, <i>t</i> , at current time-level [T].
rTop	Potential surface flux [LT ⁻¹] (infiltration/evaporation: -/+).
rRoot	Potential transpiration rate [LT ⁻¹].
vTop	Actual surface flux [LT ⁻¹] (infiltration/evaporation: -/+).
vRoot	Actual transpiration rate [LT ⁻¹].
vBot	Actual flux across the bottom of the soil profile [LT ⁻¹] (inflow/outflow: +/-).
sum(rTop)	Cumulative value of the potential surface flux [L] (infiltration/evaporation: -/+).
sum(rRoot)	Cumulative value of the potential transpiration rate [L].
sum(vTop)	Cumulative value of the actual surface flux [L] (infiltration/evaporation: -/+).
sum(vRoot)	Cumulative value of the actual transpiration rate [L].
sum(vBot)	Cumulative value of the actual flux across the bottom of the soil profile [L] (inflow/outflow: +/-).
hTop	Pressure head at the soil surface [L].
hRoot	Mean value of the pressure head over the region for which $Beta(n) > 0$ (i.e., within the root zone) [L].
hBot	Pressure head at the bottom of the soil profile [L].
RunOff	Surface runoff [LT ⁻¹].
sum(RunOff	Cumulative surface runoff [L]
Volume	Volume of water in the entire flow domain [L].
sum(Infil)	Cumulative infiltration [L]
sum(Evap)	Cumulative evaporation [L]
TLevel	Time-level (current time-step number) [-].
sum(WTran	s) Cumulative mass transfer of water between mobile and immobile regions for dual porosity model [L]

Table 13.2. RUN_INF.OUT - time and iteration information.

TLevel	Time-level (current time-step number) [-].
Time	Time, t, at current time-level [T].
dt	Time step, Δt [T].
IterW	Number of iterations necessary for solution of the water flow equation [-].
<i>IterC</i>	Number of iterations necessary for solution of the solute transport equation [-].
<i>ItCum</i>	Cumulative number of iterations [-].
KodT	Code for the boundary condition at the soil surface.
KodB	Code for the boundary condition at the bottom of the soil profile.
Converg	Information whether or not the numerical convergence was achieved at the current time-level.
Peclet	Maximum local Peclet number [-].
Courant	Maximum local Courant number [-].

Table 13.4. NOD_INF.OUT - profile information.

Node	Number of nodal point <i>n</i> .
Depth	<i>x</i> -coordinate of node <i>n</i> .
Head	Nodal value of the pressure head [L].
Moisture	Nodal value of the water content [-].
K	Nodal value of the hydraulic conductivity [LT ⁻¹].
C	Nodal value of the hydraulic capacity [L ⁻¹].
Flux	Nodal value of the Darcian velocity [LT ⁻¹].
Sink	Nodal value of the root water uptake [T ⁻¹].
Ks/KsTop	Ratio between the local hydraulic conductivity and the saturated hydraulic conductivity at the soil surface [-].
v/KsTop	Ratio between the local velocity and the saturated hydraulic conductivity at the soil surface [-].
Тетр	Nodal value of the temperature [K].
<i>Conc</i> (1,, <i>NS</i>)	Nodal value of the concentration [ML $^{-3}$]. Only given when $lChem$ =.true.
Sorb(1,,NS)	Nodal value of the sorbed concentration [MM³] or concentration in the immobile regions [ML⁻³]. Only given when <i>lChem</i> =.true. and <i>lEquil</i> =.false

The following information is printed when dual-porosity models are used.

WTrans	Water mass transfer between mobile and immobile regions [T-1].
Im.Moist.	Water content in the immobile region [-].
STrans	Solute mass transfer between mobile and immobile regions [T ⁻¹]. Only given when <i>lChem</i> =.true.

Table 13.5. BALANCE.OUT - mass balance variables.

Area	Length of the entire flow domain or a specified subregion [L].
W-Volume	Volume of water in the entire flow domain or in a specified subregion [L].
InFlow	Inflow/outflow to/from the entire flow domain or a specified subregion [LT ⁻¹].
hMean	Mean pressure head in the entire flow domain or a specified subregion [L].
TVol	Amount of heat in the entire flow domain or a specified subregion [MT ⁻²].
TMean	Mean temperature in the entire flow domain or a specified subregion [K].
COVol	Volume of CO ₂ in the entire flow domain or in a specified subregion [L ³ L ⁻²].
COMean	Mean CO ₂ concentration in the entire flow domain or in a specified subregion [L ³ L ⁻³].
ConcVol	Amount of solute in the entire flow domain or a specified subregion $[ML^{-2}]$ excluding <i>ConcVolIm</i> . This variable is given for all solutes from 1 to NS .
ConcVolIm	Amount of solute in the entire flow domain, or in a specified subregion, either adsorbed at type-2 (kinetic) adsorption sites or in the immobile liquid region $[ML^{-2}]$. This variable is given for all solutes from 1 to NS .
cMean	Mean concentration in the entire flow domain or a specified subregion $[ML^{-3}]$. This variable is given for all solutes from 1 to NS .
Top Flux	Actual surface flux [LT ⁻¹] (infiltration/evaporation: -/+).
Bot Flux	Actual flux across the bottom of the soil profile [LT ⁻¹] (inflow/outflow: +/-).
WatBalT	Absolute error in the water mass balance of the entire flow domain [L].
WatBalR	Relative error in the water mass balance of the entire flow domain [%].
The following	information is printed when carbon dioxide transport is considered.
CO2BalT	Absolute error in the CO ₂ mass balance for the entire flow domain [L].
CncBalT	Absolute error in the solute mass balance of the entire flow domain $[ML^{-2}]$. This variable is given for all solutes from 1 to NS .
CncBalR	Relative error in the solute mass balance of the entire flow domain $[\%]$. This variable is given for all solutes from 1 to NS .
The following	information is printed when dual-porosity models are used.
W-VolumeI	Volume of water in the immobile domain of the entire flow domain or a specified subregion [L].
cMeanIm	Mean concentration in the immobile domain of the entire flow domain or a specified subregion [ML 3]. This variable is given for all solutes from 1 to NS .

Table 13.6. A_LEVEL.OUT - pressure heads and cumulative fluxes on the boundary and in the root zone.

Time	Time, t, at current time-level [T].
sum(rTop)	Cumulative potential surface flux [L] (infiltration/evaporation: -/+).
sum(rRoot)	Cumulative potential transpiration [L].
sum(vTop)	Cumulative value of the actual surface flux [L] (infiltration/evaporation: -/+).
sum(vRoot)	Cumulative value of the actual transpiration [L].
sum(vBot)	Cumulative value of the bottom boundary flux [L] (inflow/outflow: +/-).
hTop	Pressure head at the soil surface [L].
hRoot	Mean value of the pressure head in the soil root zone for which Beta(n)>0 [L].
hBot	Pressure head at the bottom of the soil profile [L].
ALevel	A-level number (current variable boundary condition number) [-].