HYDRUS

One-Dimensional Variably Saturated Flow and Transport Model, Including Hysteresis and Root Water Uptake

Version 3.2

October 1989

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This report describes the one-dimensional subsurface flow and transport code HYDRUS. HYDRUS is a descendant of the program WORM developed by Dr. M. Th. van Genuchten at the USDA-ARS Salinity lab in Riverside, CA. HYDRUS is a public domain code and may be used freely. HYDRUS has been tested on a variety of flow and transport problems and has been found to work correctly. However, no warranty is given that the code is completely error-free. No liability is assumed for any losses that may result from use of the code.

If you do encounter any problems with, or find errors in the code, please contact:

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1. INTRODUCTION

1.1 General

This report is intended as documentation and user's manual for the program HYDRUS. HYDRUS simulates one-dimensional variably saturated water flow and solute transport in porous media. The solution of the flow problem considers effects of hysteresis in soil hydraulic properties and root water uptake. The solute transport equation incorporates effects of dispersion, linear or nonlinear equilibrium adsorption and first-order decay reactions. Boundary conditions for flow and transport may be constant or time-varying. For constant flow boundary conditions, HYDRUS can solve the steady-state flow equation in a single step without need to perform time marching. HYDRUS is written in FORTRAN-77 and employs fully implicit, Galerkin finite element solutions of the governing flow and transport equations.

HYDRUS is a modification of the program WORM, developed by M.Th. van Genuchten at the USDA-ARS Salinity Lab (van Genuchten, 1987). The HYDRUS routines which solve the flow and transport equations are adapted from those used in WORM. HYDRUS in addition, has the capability to model effects of hysteresis and nonlinear sorption, can accommodate variable nodal spacings, allows more flexibility in boundary conditions and has expanded input and output options.
1.2 Assumptions and Limitations

HYDRUS contains both variably saturated flow and single species solute transport models. Major assumptions of the flow model are as follows:

- Flow of the fluid phase is one-dimensional and considered isothermal and governed by Darcy's law.
- The effect of the air phase or solid-liquid interactions on water movement are considered negligible.
- The soil can be modeled as a porous medium; the presence of cracks and/or macropores is ignored.

Major assumptions of the solute transport model are as follows:

- Advection and dispersion are one-dimensional.
- Fluid properties are independent of concentration.
- Diffusive/dispersive transport is governed by Fick's law.
- Adsorption of the solute may be described by the Freundlich equilibrium isotherm; kinetic sorption processes are ignored.
- Decay of the solute may be described as a first-order process with separate rate constants for the dissolved and adsorbed phase.
2. Governing Equations

2.1 Variably Saturated Flow

The governing equation for one-dimensional, vertical flow through a rigid porous medium is

\[
C \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K \frac{\partial h}{\partial z} - K \right] - S(z,t)
\]  

(1)

where \( h \) is the pressure head (L); \( C = \partial \theta / \partial h \) is the soil water capacity (L\(^{-1}\)), \( \theta \) the volumetric water content (L\(^3\)T\(^{-3}\)); \( K \) the hydraulic conductivity (LT\(^{-1}\)); \( S(x,t) \) represents the volumetric root water uptake rate (LT\(^{-1}\)) which will be discussed later; \( z \) is soil depth which is taken to increase downward (L) and \( t \) is time (T).

Solution of (1) requires specification of the initial condition which can be given either in terms of pressure head, or in terms of water content

\[
h(z,0) = h_i(z), \quad (2a)
\]

\[
\theta(z,0) = \theta_i(z). \quad (2b)
\]

In case (2b) is used, the initial water contents are converted to initial pressure heads using the specified \( \theta(h) \) relation. A somewhat more complicated situation arises when the \( \theta(h) \) relation exhibits hysteresis. This situation is discussed in section 2.1.2.
Either first- or second-type boundary conditions can be imposed at the soil surface \((z=0)\)

\[
h(0,t) = h_0(t) \quad (3a)
\]
or

\[
\left[ -K \frac{\partial h}{\partial z} + K \right]_{z=0} = q_0(t) \quad (3b)
\]

where \(h_0(t)\) and \(q_0(t)\) are the prescribed pressure head and net fluid flux, respectively. Note that a positive flux corresponds to downward flow, and a negative flux to upward flow.

Alternatively, the upper boundary condition may be specified in terms of the total amount of surface applied water, \(Q_0 (L^3L^{-2})\). In this case, a combination of (3a) and (3b) is used by HYDRUS

\[
h(0,t) = 0 \quad t_1 < t \leq t_f \quad (4a)
\]

and

\[
\left[ -K \frac{\partial h}{\partial z} + K \right]_{z=0} = 0 \quad t_1 \geq t_f \quad (4b)
\]

where \(t_1\) is the time at which infiltration starts and \(t_f\) is the time at which the amount of infiltrated water, \(Q_{in}\), equals \(Q_0\)

\[
Q_{in} = \int_{t_1}^{t_f} q(0,t) \, dt. \quad (5)
\]

To obtain an accurate value for \(Q_{in}\) in the numerical solution, the time step, \(\Delta t\), during the period \(t_1 < t \leq t_f\) is constrained to be

\[
\Delta t \leq \min(\Delta t_{\text{max}}, 0.1Q_0/K_{s1}), \quad (6)
\]

where \(\Delta t_{\text{max}}\) is the user-specified maximum value for \(\Delta t\), and \(K_{s1}\) is the saturated conductivity of the upper soil layer.
Specifying a pulse-type boundary condition is thus equivalent to having infiltration at such a rate that the soil surface is saturated until all applied water has infiltrated, after which the boundary condition changes to a zero-flux boundary condition.

Boundary conditions for the lower soil boundary \((z=\ell)\) are

\[
\begin{align*}
h(\ell, t) &= h_\ell(t) \\
\left[ -K \frac{\partial h}{\partial z} + K \right]_{z=\ell} &= q_\ell(t) \\
\frac{\partial h}{\partial z} \bigg|_{z=\ell} &= 0
\end{align*}
\]

where \(h_\ell(t)\) and \(q_\ell(t)\) are the imposed pressure head and net drainage flux, respectively. Boundary condition \((7c)\) is equivalent to a freely draining soil profile.

The user should take note that HYDRUS uses the convention that downward flow has a positive sign and upward flow has a negative sign. This convention also applies to the infiltration rate at the soil surface and to the drainage rate at the lower boundary. A negative infiltration rate thus indicates evaporation and a negative drainage rate indicates upward flow into the soil profile.

The change from \((4a)\) to \((4b)\) is entirely under program control. Other boundary condition changes can be specified by the user by giving the appropriate boundary condition values (pressure head, flux) at selected times, in the data input file. HYDRUS allows both continuously changing (piece-wise linear in time), or step-wise changing boundary conditions.
HYDRUS assumes that the soil hydraulic properties, $\theta(h)$ and $K(\theta)$, are described by parametric functions of the form (van Genuchten, 1978)

$$\theta = \theta_s + (\theta_s - \theta_r) \left[1 + \left|ah^{-\beta}\right|^{1-\gamma}\right]^{-\gamma}$$  \hspace{1cm} (8)

$$K = K_s \frac{1}{S_e^{\frac{1}{3}}(1 - (1 - S_e^{\frac{1}{3}})^\gamma)^2}$$ \hspace{1cm} (9)

with

$$S_e = \frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} \text{ and } \gamma = 1 - \frac{1}{\beta},$$

where $\theta_s$ is the saturated water content ($L^3/L^3$), $\theta_r$ is the residual water content ($L^3/L^3$), $K_s$ is the saturated hydraulic conductivity ($L/T$), and $a$ (1/L) and $\beta$ are shape parameters. Note that the unit used for $a$ must be the reciprocal of the unit used for pressure head. Examples of typical $\theta(h)$ and $K(\theta)$ curves are shown in Figure 2.1a and 2.1b, respectively.

2.1.1 Root Water Uptake

The uptake of water by plant roots is incorporated in HYDRUS through the sink term, $S(z,t)$, in the governing flow equation (1). As modeled in HYDRUS, $S$ is determined by the potential evapotranspiration rate, $E_P$, the normalized root uptake distribution function, $t'(z)$, and a pressure-salinity stress function, $\sigma(h,h_o)$, as

$$S(z,t) = E_P(t) t'(z) \sigma(h,h_o)$$ \hspace{1cm} (10)

where $h_o$ is the osmotic head. This osmotic head is related to the solute concentration, $c$, via

$$h_o = a_1 c$$ \hspace{1cm} (11)

where $a_1$ is a simple conversion factor, the value of which depends on the units used to express pressure head and...
Figure 2.1  Typical soil water retention curve (a) and hydraulic conductivity curve (b) for Bandelier Tuff (van Genuchten et al. 1986). Data points are experimental data, solid lines represent fitted curves given by (9) and (9), respectively.
concentration. The stress-response function $\sigma$ in (10) is given by (van Genuchten, 1987)

$$
\sigma = \frac{1}{1 + [(h + h_0)/h_{50}]^p}
$$

(12)

where $h_{50}$ and $p$ are environmental and plant species specific parameters. $h_{50}$ represents the pressure head at which transpiration is reduced by 50%, and $p$ is a constant whose value has been found to be approximately 3.0 (van Genuchten, 1984). The total root water uptake rate, or actual evapotranspiration, is obtained by integrating $s$ over the root zone depth, $z_r$

$$
E_T(t) = \int_0^{z_r} S(z,t) \, dz
$$

(13)

The normalized uptake distribution function, $\zeta'$, in (10) is obtained as

$$
\zeta'(z) = \frac{\zeta(z)}{\int_0^{z_r} \zeta(z) \, dz}
$$

(14)

where $\zeta(z)$ is the actual uptake distribution. This uptake distribution function represents the maximum rate of water uptake per unit soil volume. Physically, it is a function of both the root density distribution and the root effectiveness. Normalizing the density distribution using (14) ensures that $\zeta'(z)$ integrates to unity over the root zone. Since the water stress factor, $\sigma$, is always less than, or equal to 1.0, it is guaranteed that
\[
\ell_r \int s(z,t)dz \leq E_p(t)
\]

In other words, the actual root uptake rate can never exceed the potential evapotranspiration rate.

2.1.2 Hysteresis in Soil Moisture Characteristic

Although the soil moisture characteristic \( \theta(h) \) is usually taken to be a single-valued function, the actual relationship for most soils exhibit hysteresis. At a given value of pressure head, water contents will be higher when the soil is drying than when the soil is wetting. An example of a hysteretic \( \theta(h) \) relation is shown in Figure 2.2. The figure shows the boundary wetting and drying curves. The wetting relationship is indicated with superscript \( \ast \), while the drying relationship is indicated with \( \d \). HYDRUS incorporates the procedure described by Kool and Parker (1977) to model hysteresis. This procedure is summarized below. To model the effect of hysteresis it is required that both the boundary wetting and the boundary drying curves are known. In HYDRUS it is assumed that then curves can be described parametrically by the van Genuchten relationship (8), but with different parameter values for the boundary wetting and drying branches. Using superscript \( \ast \) and \( \d \) for wetting and drying respectively, the boundary \( \theta(h) \) curves are then described by

**Wetting:**

\[
\frac{\theta - \theta_r}{\theta_w - \theta_r} = \left(1 + \left|\theta h\right|^n \right)^{-m} \quad h < 0
\]

\[
\frac{\theta - \theta_r}{\theta_w - \theta_r} = \left(1 + \left|\theta h\right|^n \right)^{-m} \quad h \geq 0
\]

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Drying:

\[
\frac{1}{1 + |\alpha h|^\gamma} \quad h < 0
\]

\[
\frac{1}{\hat{\psi} - \hat{\psi}_d} = \begin{cases} 
\frac{\hat{\psi}_s - \hat{\psi}_d}{1} & h \geq 0 
\end{cases}
\]

with \( \gamma^r = 1 - 1/\beta^w \) and \( \gamma^d = 1 - 1/\beta^d \)

In the above equation, \( \hat{\psi}_s \) is the saturated water content value; \( \hat{\psi}_s^* \) represents the maximum water content upon rewetting of an initially air-dry soil. If there is no air entrapment, \( \hat{\psi}_s^* = \hat{\psi}_s^d \). However, if air-entrapment occurs, \( \hat{\psi}_s^* \) will be less than \( \hat{\psi}_s^d \). Parameters \( \alpha \) and \( \beta \) are the curve shape parameters, with different values for wetting and drying. Note that \( \alpha^w \) cannot be less than \( \alpha^d \), i.e.

\[ \alpha^w \geq \alpha^d \]

Lacking data, one may use \( \alpha^w = 2\alpha^d \) as a first approximation (Kool and Parker, 1987). Furthermore, it is often justified to make the following simplification

\[ \beta^w = \beta^d = \beta. \]

Using these approximations, modeling hysteresis is parametrically no more complex than modeling non-hysteretic flow. In a hysteretic flow simulation, HYDRUS automatically computes scanning curves in the \( \theta(h) \) relation to determine the appropriate wetting or drying path for every node in the domain when reversals from drying to wetting, or vice-versa, occur. This is achieved by defining "pseudo" values for the residual and
saturated water contents at each node in the modeled domain. In the simulation, these pseudo-values are substituted into Eqs. (15a) and (15b). This has the effect of scaling the boundary wetting and drying curves to approximate the scanning curves.

Denoting the "pseudo"-values for \( \theta_e \) and \( \theta_s \) as \( \theta_e^* \) and \( \theta_s^* \), respectively, the procedure to calculate these parameters is as follows: For a wetting scanning curve \( \theta_e \) is replaced by \( \theta_e^* \), which is evaluated as

\[
\theta_e^* = \frac{\theta_e^* - \theta_s S_e \rho_e^*(h^*)}{1 - S_e \rho_e^*(h^*)}
\]  

(16)

where \( h^* \) and \( \theta^* \) are the pressure head and water content, respectively, at the latest reversal from drying to wetting. For a drying scanning curve, \( \theta_s \) is replaced by \( \theta_s^* \) which is evaluated as

\[
\theta_s^* = \frac{\theta_s^* - \theta_e \rho_e^*(h^*)}{S_e \rho_e^*(h^*)}
\]  

(17)

\( h^* \) and \( \theta^* \) again represent the pressure head and water content at the most recent reversal, this time from wetting to drying. In the above equations, \( S_e \) is the relative saturation, defined as

\[
S_e = \frac{\theta - \theta_e}{\theta_s - \theta_e}
\]  

(18)

Superscripts \( d \) and \( w \) for drying and wetting, respectively, denote evaluation using parameters for the main drying and main wetting curve, see Eq. 15a and 15b, respectively.
Figure 2.2. Example moisture retention curve with hysteresis. Shown are the boundary wetting curve, $\theta^w(h)$, and the boundary drying curve, $\theta^d(h)$.
In the case where the main hysteresis loop is not closed at saturation, i.e., \( \theta_s^d < \theta_s^w \), the water content at saturation for a wetting scanning curve, \( \theta_s^w \) in Eq. 16) is evaluated using the empirical relationship of Aziz and Settari (1979)

\[
\theta_s = \theta_s^d - \frac{\theta_s^d - \theta_r}{1 + R(\theta_s^d - \theta^w)}
\]  \hspace{1cm} (19)

with

\[
R = \frac{\frac{1}{\theta_s^d - \theta_s^w} - \frac{1}{\theta_s^d - \theta_r}}{\theta_s^d - \theta_s^w - \theta_s^d - \theta_r}
\]

The interpolation procedure defined by (19) ensures that the value for the saturated water content used for scanning curves falls in between \( \theta_s^d \) and \( \theta_s^w \). Furthermore, after several wetting-drying cycles, the saturated water content will converge to \( \theta_s^w \) to mimic the effect of increasing air entrainment.

To fully implement the above outlined scheme for modeling hysteresis, it is also necessary to track which parts of the soil profile are, at any given time, wetting and which are drying. This is achieved by assigning a simple integer index to every node in the domain. The hysteresis index, \( \kappa \), takes a value of +1 if the node is wetting (\( h_{1t}^{t+\Delta t} > h_{1t}^t \)) and a value of -1 if the node is drying (\( h_{1t}^{t+\Delta t} < h_{1t}^t \)). A check for reversals from wetting to drying or vice-versa is made at the conclusion of each time step.
2.2 Solute Transport

Transport of miscible components is described by the advection-dispersion equation

\[
\frac{\partial}{\partial z} \left( \frac{\partial c}{\partial z} \right) - q \frac{\partial c}{\partial z} - \lambda_1 \frac{\partial c}{\partial t} - \lambda_2 \frac{\partial b}{\partial t} = \frac{\partial c}{\partial t} + \rho_b \frac{\partial b}{\partial t}
\]  \hspace{1cm} (20)

where \( c \) is the solute concentration (M/L^3), \( s \) is the adsorbed concentration (M/L^3), \( D \) is the dispersion coefficient (L^2/T), \( q \) is the Darcy velocity (L/T), and \( \lambda_1 \) and \( \lambda_2 \) are first-order decay coefficients (T^{-1}), for the dissolved phase and adsorbed phase, respectively. The dispersion coefficient is defined as

\[
D = \epsilon v + D^s
\]  \hspace{1cm} (21)

where \( \epsilon \) is the dispersivity (L) of the medium, \( v = q/\epsilon \) is the average pore water velocity (L/T), and \( D^s \) is the apparent molecular diffusion coefficient (L^2/T).

Assuming the dissolved and adsorbed concentrations are in local equilibrium, the time derivative \( \delta s/\delta t \) can be written as

\[
\frac{\delta s}{\delta t} = \frac{ds}{dc} \frac{\delta c}{\delta t}
\]  \hspace{1cm} (22)

Substitution into (20) allows the governing equation to be written as

\[
\frac{\partial}{\partial z} \left( \frac{\partial c}{\partial z} \right) - q \frac{\partial c}{\partial z} - \lambda_1 \frac{\partial c}{\partial t} - \lambda_2 \rho_b \frac{\partial s}{\partial t} = \left( \frac{\partial}{\partial t} + \rho_b f \right) \frac{\partial c}{\partial t}
\]  \hspace{1cm} (23)

where \( f = ds/dc \) is the slope of the adsorption isotherm (M/L^3).
A general expression for the adsorption isotherm is given by the Freundlich isotherm

\[ s = k_1 c^\eta \]  
\[ \text{(24a)} \]

or

\[ \frac{ds}{dc} = k_1^{\eta} c^{\eta-1} \]  
\[ \text{(24b)} \]

where \( k_1 \) and \( \eta \) are coefficients. Note that when the exponent \( \eta \) equals 1, the Freundlich isotherm becomes linear, and the coefficient \( k_1 \) identical to the familiar solid-liquid phase partition coefficient, \( k_d \). When the exponent \( \eta \) is different from 1.0, the isotherm, and in turn the transport equation itself, becomes nonlinear. In this case an iterative procedure, similar to the one used to solve the unsaturated flow equation, must be used to solve the solute transport equation.

Using (24a,b) an overall decay coefficient and retardation factor can be defined as

\[ \lambda = \lambda_1 + \frac{\beta k_1 c^{\eta-1}}{\beta} \lambda_2 \]  
\[ \text{(25)} \]

\[ R = 1 + \frac{\beta k_1 c^{\eta-1}}{\beta} \]  
\[ \text{(26)} \]

The final form of the solute transport equation solved by HYDRUS can thus be written as

\[ \frac{\partial}{\partial z} \left( \frac{\partial C}{\partial z} \right) - q \frac{\partial C}{\partial t} - \lambda R \frac{\partial C}{\partial t} = 0 \]  
\[ \text{(27)} \]

Note that, unless \( \eta = 1 \), both \( \lambda \) and \( R \) are nonlinear coefficients.

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At the soil surface, either first-type or third-type boundary conditions can be specified:

\[ c(0,t) = c_0(t) \]  \hspace{1cm} (28a) \\

or

\[ \left(-\frac{\partial c}{\partial z} + qc\right)_{z=0} = \begin{cases} q_0 c_0 & q > 0 \\ 0 & q \leq 0 \end{cases} \]  \hspace{1cm} (28b)

where \( c_0 \) is the actual concentration of the soil solution at the soil surface in case (28a) is used, or \( c_0 \) is the concentration of the infiltrating water if (28b) is used, and \( q_0 \) is the Darcy flow rate at the soil surface. Note that \( q \) is taken to be positive for downward flow and negative for upward flow. Boundary condition (28b) specifies a zero efflux of solute during periods of evaporation.

A zero gradient boundary condition at \( z=\ell \) is used during periods of drainage

\[ \frac{\partial c}{\partial z} \bigg|_{z=\ell} = 0 \hspace{1cm} q_\ell > 0 \]  \hspace{1cm} (29a)

During periods of upward flow from a watertable, a first-type boundary condition is used

\[ c(\ell,t) = c_\ell(t) \]  \hspace{1cm} (29b)
3 NUMERICAL IMPLEMENTATION

3.1 Solution of the Flow Equation

HYDRUS uses the linear finite element solution of the unsaturated flow equation described by van Genuchten (1978, 1987). A summary description of the numerical scheme is given below.

The soil profile is discretized into a number of elements of size \( \Delta z \). The unknown pressure head is assumed to vary linearly across each element \([z_1, z_2]\)

\[
h(\xi, t) = \phi_1(\xi) h_1(t) + \phi_2(\xi) h_2(t) \quad -1 \leq \xi \leq 1
\]

(30)

where \( \phi_1 \) and \( \phi_2 \) are linear basis functions defined in a local coordinate system, \( \xi \), (van Genuchten, 1978) and \( h_1 \) and \( h_2 \) are the pressure heads at the nodal points \( z_1 \) and \( z_2 \) respectively.

The local coordinate is defined as (van Genuchten, 1978)

\[
\xi = \frac{2(z - z_1)}{z_2 - z_1} - 1 \quad z_1 \leq z \leq z_2
\]

(31)

Substitution of the approximation (30) into the governing equation (1), application of the Galerkin principle and integration by parts eventually leads to a matrix equation of the form

\[
[A] \{h\} + [B] \frac{d\{h\}}{dt} = \{F\}
\]

(32)

where

\[
[A_{ij}] = \int_0^t K \frac{d\phi_i}{dz} \frac{d\phi_j}{dz} dz
\]

(33a)

3-1
\[ [B_{ij}] = \int_0^\ell C \phi_i \phi_j \, dz \quad (33b) \]

\[ \{F_i\} = -q_0 \phi_i \int_0^\ell + \int_0^\ell \left( \frac{d\phi_i}{dz} - S \phi_i \right) \, dz \quad (33c) \]

The nonlinear coefficients \( K \) and \( C \) are interpolated linearly across each element, analogous to the pressure head

\[ K(\xi) = \phi_1(\xi)K_1 + \phi_2(\xi)K_2 \quad (34a) \]

\[ C(\xi) = \phi_1(\xi)C_1 + \phi_2(\xi)C_2 \quad (34b) \]

where \( \xi \) is the local coordinate \((-1 \leq \xi \leq 1)\) and \( K_1, K_2, C_1, \) and \( C_2 \) are the nodal values of the respective coefficients. The same interpolation is used also for the root uptake term \( S \)

\[ S(\xi) = \phi_1(\xi)S_1 + \phi_2(\xi)S_2 \quad (34c) \]

where \( S_1 \) and \( S_2 \) are nodal values of \( S \).

To speed up convergence of the iterative numerical solution, mass lumping is applied to the matrix \([B]\). To achieve this the terms involving time derivatives are redefined using

\[ \int_0^\ell C \frac{\partial h}{\partial t} \phi_i \, dz = \frac{\partial h}{\partial t} \int_0^\ell C \phi_i \, dz \quad (35) \]

The mass-lumped finite element scheme can be further simplified by redefining the time derivative terms (van Genuchten, 1978)
\[
\frac{\delta h}{\delta t} \int_0^\ell \frac{\delta h}{\delta t} \phi_1 dz = \frac{\delta h}{\delta t} \int_0^\ell \phi_1 dz
\]  

(36)

Applying mass lumping according to (36) is equivalent to using a finite difference solution scheme (van Genuchten, 1978). To distinguish the two mass lumping options, we use the terminology of Milly (1985). Mass lumping scheme (35) is referred to as the 'L_1 - scheme', while mass lumping according to (36) is referred to as the 'L_2 - scheme'.

The time derivative in (30) is approximated by a simple finite difference scheme, using the following approximations

\[
\frac{d(h)^{t+\Delta t}}{dt} = \frac{(h)^{t+\Delta t} - (h)^t}{\Delta t}
\]  

(37a)

\[
(h)^{t+\Delta t} = \omega(h)^{t+\Delta t} + (1-\omega)(h)^t
\]  

(37b)

where \( \omega \) is a temporal weighting coefficient (0 \leq \omega \leq 1). By defining the matrix equation (32) at the half-time level (\( t+\frac{1}{2}\Delta t \)) and using (37a) and (37b), the following set of equations is obtained:

\[
[P]^t+\frac{1}{2}\Delta t (h)^{t+\frac{1}{2}\Delta t} = [Q]^t+\frac{1}{2}\Delta t (h)^t + [F]^t+\frac{1}{2}\Delta t
\]  

(38)

where

\[
[P] = \omega[A] + \frac{1}{\Delta t} [B]
\]  

(39a)

\[
[Q] = (1-\omega)[A] + \frac{1}{\Delta t} [B]
\]  

(39b)

Although the temporal weighting coefficient \( \omega \) can in principle take any value between 0 and 1, in practice either \( \omega = 0.5 \) or
\( \omega = 1 \) is used. When \( \omega = 0.5 \) a Crank-Nicholson scheme is obtained. When \( \omega = 1 \), a fully implicit or backward difference scheme is obtained. Although the Crank-Nicholson approximation is of higher order than the fully implicit approximation, the Crank-Nicholson scheme is often prone to numerical oscillations, particularly when steep moisture fronts are simulated. For this reason, HYDRUS uses the fully implicit scheme. Using \( \omega = 1 \), Equation (38) can be expanded as follows for the i-th node:

\[
a h_{i-1}^{t+\Delta t} + b h_{i}^{t+\Delta t} + c h_{i+1}^{t+\Delta t} = f
\]

(40)

where

\[
a = \frac{-1}{2\Delta z_{i-1}} (K_{i-1} + K_{i})
\]

(41a)

\[
b = \frac{1}{2\Delta z_{i-1}} (K_{i-1} + K_{i}) + \frac{1}{2\Delta z_{i}} (K_{i} + K_{i+1}) + \frac{\Delta z_{i-1}}{6\Delta t} (C_{i-1} + 2C_{i}) + \frac{\Delta z_{i}}{6\Delta t} (2C_{i} + C_{i+1})
\]

(41b)

or

\[
b = \frac{1}{2\Delta z_{i-1}} (K_{i-1} + K_{i}) + \frac{1}{2\Delta z_{i}} (K_{i} + K_{i+1}) + \frac{\Delta z_{i-1}}{2\Delta t} C_{i} + \frac{\Delta z_{i}}{2\Delta t} C_{i}
\]

(41c)

\[
c = \frac{-1}{2\Delta z_{i}} (K_{i} + K_{i+1})
\]

(41d)

\[
f = h_{i}^{t} \left[ \frac{\Delta z_{i-1}}{6\Delta t} (C_{i-1} + 2C_{i}) + \frac{\Delta z_{i}}{6\Delta t} (2C_{i} + C_{i+1}) \right] + \frac{3-4}{2}
\]
\[ \frac{1}{2} (K_{i-1} - K_{i+1}) - \frac{\Delta z_{i-1}}{6}(S_{i-1} + 2S_i) - \frac{\Delta z_i}{6}(S_i + S_{i+1}) \quad (41e) \]

or

\[ f = h_1^t \left[ \frac{\Delta z_{i-1}}{2\Delta t} C_i + \frac{\Delta z_i}{2\Delta t} C_i \right] + \frac{1}{2}(K_{i-1} - K_{i+1}) - \frac{\Delta z_{i-1}}{6}(S_{i-1} + 2S_i) - \frac{\Delta z_i}{6}(2S_i + S_{i+1}) \quad (41f) \]

where \( \Delta z_{i-1} \) and \( \Delta z_i \) are the nodal spacings for the elements adjoining node \( i \). Coefficients \( b \) and \( f \) are given by (41b) and (41e), respectively, if the \( L_1 \) mass-lumping scheme is used. If the \( L_2 \)-scheme is used, the coefficients \( b \) and \( f \) are given by (41c) and (41f), respectively.

3.1.1 Time stepping procedure and handling of nonlinear coefficients.

Since the hydraulic conductivity and capacity in (1) are both nonlinear functions of pressure head, \( h \), iteration is required at every time step to reach the correct solution, i.e., the nodal values of pressure head at the new time level. HYDRUS uses the Picard iteration method with underrelaxation as described by Cooley (1983). Convergence is achieved if the following condition is satisfied

\[ |h_{1}^{t+\Delta t} - h_{1}^{t+\Delta t}| \leq r_1 + r_2 |h_{1}^{t+\Delta t}| \quad (42) \]

where \( h_{1}^{t+\Delta t} \) and \( h_{1}^{t+\Delta t} \) are the projected and computed value of pressure head at the \( i \)-th node for the new time level, respectively, and \( r_1 \) and \( r_2 \) are absolute and relative convergence criteria. HYDRUS automatically updates the value of the time step, \( \Delta t \), depending on how quickly the solution converged at the

1-5
previous time step, using the following rules:

\[
\Delta t_{n+1} = \min(1.25 \Delta t_n, \Delta t_{\text{max}}) \quad \text{if } k \leq 2 \tag{43a}
\]
\[
\Delta t_{n+1} = 0.8\Delta t_n \quad \text{if } k \geq 6 \tag{43b}
\]

Where \( n \) denotes time step and \( k \) is the number of iterations at the \( n \)-th timestep.

At the beginning of a new time step an estimate of the new pressurehead value is obtained by linear interpolation from the current and previous pressure head values

\[
h_t^{n+1} = h_t^n + \frac{\Delta t_{n+1}}{\Delta t_n} (h^n - h_{n-1}) \tag{44}
\]

Both convergence and accuracy of the flow solution are strongly influenced by how the nonlinear hydraulic conductivity and capacity, \( K \) and \( C \), respectively, in Eq (1) are evaluated. Particularly when steep moisture gradients are present, proper evaluation of the capacity \( C \) has a pronounced effect on mass balance accuracy. Numerical flow solutions using the pressure head formulation are often prone to significant mass balance errors when scenarios involving steep moisture fronts are simulated. For these problems, solution schemes using water content as dependent variable have been proposed (e.g., Hills et al., 1989) since this formulation is inherently mass conservative.

As pointed out by Milly (1985), it is possible to obtain a mass-conservative flow solution using the head based formulation, provided the capacity terms are evaluated in an appropriate manner. In this way, a mass-conservative solution can be guaranteed for any spatial or temporal discretization. In order to achieve this, the moisture capacity is defined such that at
the element level the following equality holds

\[ \int_e c_e (h^{t+\Delta t} - h^t) \, de = \int_e (s^{t+\Delta t} - s^t) \, de \]  

(45)

where \( c_e \) is the effective element moisture capacity given by (34b) and integration is performed on an element by an element basis. The resulting expressions for the nodal values of \( C \) depend on the formulation of the mass-matrix \( [B] \) in (32). When \( [B] \) is formulated according to the \( L_1 \) mass-lumping scheme, see (35), the nodal values of \( C \) are given by (Milly, 1985)

\[ c_{ej} = \frac{\Delta s^t_j \int \phi_j \, de}{2 \Delta h \sum_{m=1}^2 \phi_j \phi_m \, de} \]  

(46)

which leads to

\[ c_{e1} = \frac{3\Delta s^t_1}{2\Delta h_1^t + \Delta h_2^t} \]  

(47a)

\[ c_{e2} = \frac{3\Delta s^t_2}{\Delta h_1^t + 2\Delta h_2^t} \]  

(47b)

where \( \Delta s^t_1 = s_1^{t+\Delta t} - s_1^t \) and \( \Delta h_1^t = h_1^{t+\Delta t} - h_1^t \).
The nodal capacity values in this scheme are discontinuous at element boundaries. A simpler scheme results when the mass matrix [B] is diagonalized according to the L2-scheme, see (36). In this case, the nodal capacity values are continuous at element boundaries and given by the following secant formula

$$C_i = \frac{\Delta t}{\Delta h_i} \quad (i = 1, \ldots, n) \quad (48)$$

When nodal pressure head changes are very small, the denominator in both (46 a,b) and (47) will tend to zero. When this happens the moisture capacity is computed analytically as the derivative of the soil moisture characteristic, see Eq. (8), evaluated at the half-time level

$$h^{t+\frac{1}{2} \Delta t} = \frac{1}{2} (h^t + h^{t+\Delta t})$$

$$C_i = \frac{d \theta(h)}{dh} \bigg|_{h_i^{t+\frac{1}{2} \Delta t}} \quad (49)$$

In HYDRUS, nodal values of hydraulic conductivity are always evaluated at the half-time level using Eq. (9).

$$K_i = K(h_i^{t+\frac{1}{2} \Delta t}) \quad (50)$$

In situations involving steep moisture fronts and/or highly nonlinear soil hydraulic properties, behavior of the numerical flow solution can sometimes be improved by applying upstream weighting to the hydraulic conductivity. This is achieved by redefining (33a) as

$$K(\xi) = (1 + \delta)\phi_1(\xi)K_1 + (1 - \delta)\phi_2(\xi)K_2 \quad (51)$$
where $\delta$ is a weighting coefficient with $0 \leq |\delta| \leq 1$. The sign of $\delta$ is positive if the direction of flow is from node 1 to node 2, and negative if flow is in the reverse direction. When the optional upstream weighting is selected, HYDRUS always uses full upstream weighting ($\delta = \pm 1$).

Nonheterogeneous soil properties are accommodated in HYDRUS by simply evaluating nodal values of the coefficients $K$ and $C$ using the hydraulic parameters that are appropriate for that particular nodal location.

3.2 Solution of the Solute Transport Equation

The solute transport equation (27) is solved using the Galerkin linear finite element method. The solution procedure parallels the one for the flow equation. The dependent variable, i.e., concentration $c(z,t)$, is approximated by a piece-wise linear function

$$c(z,t) = \sum_{j=1}^{n} \phi_j(z)c_j(t)$$  \hspace{1cm} (52)

Application of the Galerkin method to the spatial terms with finite difference approximation of the time derivative eventually leads to the following matrix equation

$$\omega[A][\{c\}^{t+\Delta t}] + \frac{1}{\Delta t}[B](\{c\}^{t+\Delta t} - \{c\}^t) = \{F\} + (\omega - 1)\{c\}^t$$  \hspace{1cm} (53)

where $\omega$ is again the time weighting coefficient. Setting $\omega = \frac{1}{2}$, i.e., using a Crank-Nicholson scheme, leads to a second-order correct solution, but often produces oscillations in the computed concentration profile. Such oscillations can be avoided by setting $\omega = 1$, but at the expense of a smeared concentration front when $D/v$ is relatively small. To overcome the latter
problem, van Genuchten (1978) developed correction factors to be applied to the dispersion coefficient. This solution is used in HYDRUS. Following the development of van Genuchten (1978, 1987) the final matrix equation is

\[ [P]^{t+\Delta t} [c]^{t+\Delta t} = [Q]^{t} [c]^{t} + [F] \]  

(54)

where

\[ [P_{ij}] = \int_{0}^{\ell} \left[ \frac{1}{2} \left( \langle D_{-} \frac{d\phi}{dz} - q_{\phi} \rangle \frac{d\phi}{dz} + \langle \frac{dR}{\Delta t} - \frac{\lambda}{2} \rangle \phi \right) \right] dz \]  

(55a)

\[ [Q_{ij}] = \int_{0}^{\ell} \left[ \frac{-1}{2} \left( \langle D_{+} \frac{d\phi}{dz} - q_{\phi} \rangle \frac{d\phi}{dz} + \langle \frac{dR}{\Delta t} - \frac{\lambda}{2} \rangle \phi \right) \right] dz \]  

(55b)

\[ \{F\} = \frac{1}{2} \left( q_{s}^{t+\Delta t} + q_{s}^{t} \phi \right) \]  

(55c)

\[ q_{s} = -\langle D_{+} \frac{d\phi}{dz} + q_{s} \phi \rangle \]  

(55d)

The coefficients \( D_{-} \) and \( D_{+} \) in (55a) and (55b) represent the dispersion correction factors and are given by

\[ D_{-} = D - \frac{q_{s}^{2} \Delta t}{6s_{R}} \quad D_{+} = D + \frac{q_{s}^{2} \Delta t}{6s_{R}} \]  

(56)

Note that \( D_{-} \) and \( D_{+} \) are evaluated at the new and old time levels, i.e., using the previous and current values of \( q \) and \( \phi \), respectively.

Upon solving the integrals in (55), a tridiagonal matrix \([P]\) is
obtained. Let $b$, $d$, and $a$ represent the below-diagonal, diagonal, and above-diagonal terms of $[P]$, respectively. These terms are given by

$$b_i = \frac{-1}{4\Delta x_{i-1}}(\delta_{i-1}^+ D_{i-1}^+ + \delta_{i}^- D_i^-) - \frac{1}{12}(2q_{i-1} + q_i) \quad (57a)$$

$$d_i = \frac{-1}{4\Delta x_{i-1}}(\delta_{i-1}^- D_{i-1}^- + \delta_{i}^+ D_i^+) + \frac{1}{4\Delta x_i} (\delta_{i}^- D_i^- + \delta_{i+1}^- D_{i+1}^-) + \frac{\Delta x_{i-1}}{6\Delta t}(\delta_{i-1}^+ U_{i-1} + 2\delta_{i}^+ U_i) + \frac{\Delta x_i}{6\Delta t}(2\delta_{i}^+ U_i + \delta_{i+1}^+ U_{i+1}) + \frac{\lambda}{12}(q_{i+1} - q_{i-1}) \quad (57b)$$

$$a_i = \frac{-1}{4\Delta x_i} (\delta_{i}^+ D_i^+ + \delta_{i+1}^+ D_{i+1}^+) + \frac{1}{12}(q_i + 2q_{i-1}) \quad (57c)$$

with

$$U_i = R_i - \frac{\lambda \Delta t}{2} \quad (57d)$$

The entries of matrix $[Q]$ are the same as those of $[P]$ except that $D^-$ is replaced by $-D^+$, $q$ is replaced by $-q$, and $\lambda$ is replaced by $-\lambda$. The vector $(F)$ in (54) is given by

$$f_1 = \frac{1}{2} [q_B(0,t+\Delta t) + q_B(0,t)] \quad (58a)$$

$$f_i = 0 \quad 2 \leq i \leq n-1 \quad (58b)$$

$$f_n = \frac{1}{2} [q_B(t,t+\Delta t) + q_B(t,t)] \quad (58c)$$
4 VERIFICATION AND VALIDATION PROBLEMS

This section presents a number of problems designed to show verification and validation of the HYDRUS code. The selected problems involve flow as well as solute transport examples, and range from controlled laboratory experiments to field problems. The following problems are included:

- Infiltration and drainage in a large caisson of crushed tuff.
- Transient flow in a laboratory column involving hysteresis in the soil hydraulic properties.
- Metal transport involving ion exchange reactions, under steady state flow conditions.

4.1 Infiltration and Drainage in a Large Caisson.

The first problem involves transient infiltration and drainage of water in a large caisson. The experimental study was conducted at Los Alamos National Laboratory in order to investigate the hydraulic properties of Bandelier Tuff. The tuff is the principal rock type exposed in the Los Alamos area. Radioactive wastes have been disposed of in pits and trenches excavated in the surface of the Bandelier Tuff since the 1940's (Abeele et al., 1981). Design and data collection of the caisson experiment are described in Abeele (1984). The caisson measured 6m in depth by 3m diameter. The caisson was filled with crushed Bandelier Tuff and instrumented with a number neutron probe access tubes for measuring water contents, installed horizontally from the outside of the caisson at different depths, as well as tensiometers for measuring soil water potentials, installed at the same depths. The initially dry tuff in the caisson was first saturated with water and then allowed to drain under gravity.
The caisson surface was covered during drainage to prevent evaporation. The moisture retention characteristic was obtained from simultaneous measurements of pressure head and water content. The hydraulic conductivity function was determined from water content measurements during drainage using the instantaneous profile method. These hydraulic relationships of the Bandelier Tuff are shown as the data points in Figure 1.1a and 1.1b, respectively. The solid lines in these figures represent the van Genuchten relations, see Eqs. (8) and (9), fitted to the measured data. Hydraulic parameter values are given in Table 4.1. Note that the data shown in Figure 1.1 correspond to drying curves. Hysteresis is ignored in this analysis.

First, wetting of the caisson is modeled. The Bandelier Tuff was assumed to be at a uniform initial water content of 10% by volume. The caisson was wetted by applying water at a rate of 20 cm/d for 5 days. After 5 days the caisson was further wetted to complete saturation by ponding. The infiltration of water into dry soil represents a numerically difficult problem, the solution of which may encounter slow convergence and sometimes substantial mass balance errors (e.g., Hills et al., 1989). Simulating wetting of the caisson thus represent a good test of the accuracy and numerical robustness of the unsaturated flow solution in HYDRUS. For the flow simulation, the 6 m deep caisson was discretized into 120 elements of uniform length, corresponding to a nodal spacing of 5 cm. Absolute and relative pressure head converge tolerances were set to values of 1 cm and 1%, respectively. The simulation was performed using the mass conservative flow solution scheme with evaluation of nodal capacities according to (48). For comparison purposes, the simulation was also performed using HYDRUS with an alternative scheme in which the nodal capacities were evaluated analytically as the derivatives of the moisture retention function, Eq (8).
This latter scheme is commonly used in unsaturated flow models, but does not ensure conservation of mass.

Both simulations were performed on a 25 MHz 80386 personal computer. Results are presented in Table 4.2 and Figure 4.1, respectively. Table 4.2 shows a comparison of cumulative mass balance errors and execution times. Figure 4.1 presents computed water content profiles after 2, 4 and 6 days for the two simulations. Table 4.2 indicates that when the non-mass conservative flow solution is used, the mass balance error increases with time. After 7 days, the relative error is greater than 8% of the total amount of water in the caisson. The predicted wetting front obtained using the non-mass conservative scheme consistently lags behind the wetting front obtained with the mass conservative solution. When the mass conservative flow solution is used, the mass balance errors in HYDRUS are less than 1% at all times and actually decrease with time. The results in Table 4.2 indicate that the CPU requirements of the different solution schemes are comparable. The second part of this first test problem involves simulation of the caisson drainage. Gravity drainage commenced following complete saturation of the caisson. Drainage in simulated using a zero flux boundary condition at the caisson surface and a zero pressure head condition at the base of the caisson. Nodal spacing and convergence tolerances were set to the same values as used in the infiltration simulation. Drainage was simulated for a period of 100 days using HYDRUS with the \( L_1 \) - mass lumping scheme. CPU requirements and mass balance results are shown in Table 4.3. Predicted moisture profiles in the caisson after \( t = 1, 4, 20 \) and 100 days of drainage are compared to measured water content data in Figure 4.2.
Table 4.1 Hydraulic parameters of crushed Bandelier Tuff used in caisson experiments. Parameters correspond to van Genuchten relationships, see Eqs. (8) and (9).

<table>
<thead>
<tr>
<th>Hydraulic Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>εs</td>
<td>-</td>
<td>0.3308</td>
</tr>
<tr>
<td>εr</td>
<td>-</td>
<td>0.0</td>
</tr>
<tr>
<td>α</td>
<td>cm⁻¹</td>
<td>0.01433</td>
</tr>
<tr>
<td>β</td>
<td>-</td>
<td>1.506</td>
</tr>
<tr>
<td>Ks</td>
<td>cm/d</td>
<td>25.0</td>
</tr>
</tbody>
</table>
Table 4.2  Mass balance errors and CPU times for simulation of caisson infiltration.

<table>
<thead>
<tr>
<th></th>
<th>Mass Conservative</th>
<th>Analytical</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C(h)</td>
<td>C(h)</td>
</tr>
<tr>
<td>mass balance error (%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 days</td>
<td>0.96</td>
<td>4.97</td>
</tr>
<tr>
<td>4 days</td>
<td>0.80</td>
<td>6.83</td>
</tr>
<tr>
<td>7 days</td>
<td>0.67</td>
<td>8.28</td>
</tr>
<tr>
<td>No. of time steps</td>
<td>1093</td>
<td>1038</td>
</tr>
<tr>
<td>CPU time (sec)</td>
<td>631.6</td>
<td>532.4</td>
</tr>
</tbody>
</table>
Figure 4.1 Predicted water content profiles during transient infiltration in Bandelier Tuff. —
The 100 day drainage simulation required only 130 timesteps and 63 seconds of CPU time. This is in marked contrast to the much greater computational requirements of the 7 day infiltration simulation and illustrates again the relative difficulty of simulating the infiltration problem. The comparison of observed and simulated water content profiles in the caisson during drainage show good agreement. Upon inspection, it can be seen that the initial drainage from the caisson is overpredicted, resulting in somewhat lower predicted than observed water contents after 1 day. At subsequent times however, the predicted water content profiles agree very closely with the measured data.

4.2 Unsaturated Flow with Hysteresis

The second test problem is designed to test the ability of HYDRUS to simulate unsaturated flow involving a hysteretic moisture retention characteristic. The problem examined is a column experiment described by Gillham et al. (1979). The experiment was performed on a 60 cm tall, vertical column of Dune sand, which was initially water-saturated. The column was first partially drained, followed by rewetting. Flow was controlled by manipulating the pressure head at the base of the column. The hysteretic moisture retention characteristic of the Dune sand was determined by Gillham et al. (1979) using tensiometers and a gamma ray apparatus. To model this experiment, the van Genuchten water retention function was used. The measured and fitted water retention curves of the Dune sand are shown in Figure 1.2. Data points represent the experimental data of Gillham et al. (1979). The fitted van Genuchten curve is shown as the solid line. It can be seen that the van Genuchten function very accurately describes the experimental data. Best-fit values of the van Genuchten parameters for the Dune sand are presented in Table 4.4. The unsaturated hydraulic conductivity–water content
Figure 4.2 Predicted and observed water content profiles during drainage of Bandelier Tuff. Data points from Abeels et al. (1984).
relation of the Dune sand was found by Gillham et al. (1979) to be described by the following functional relationship:

$$K = K_S \left(\frac{-\theta}{\theta_s}\right)^{5.509}$$

In modeling the transient flow experiment, this $K(\theta)$ relation was used together with the van Genuchten relationship for the main drying and wetting boundary curves in the $\theta(h)$ relation. The water content distribution inside the column was measured at $t = 68$ minutes, and $t = 125$ minutes after the start of the experiment. Computed water content profiles are compared against these measured data in Figure 4.3. At the first time value ($t = 68$ mins) the entire column is draining along the main drainage branch. At $t = 125$ mins most of the column is being resaturated again with upward flow from the base of the column were still draining at this time. The figure shows very good agreement between observed and simulated water content profiles at both time values, there by illustrating the efficacy of the hysteresis algorithm implemented in HYDRUS. Further examples of flow simulations involving hysteresis can be found in Kool and Parker (1987).
Table 4.4 Hydraulic parameters of Dune sand used in modeling column flow experiment.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_s$</td>
<td>cm/hr</td>
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</tr>
<tr>
<td>$\theta_d$</td>
<td>-</td>
<td>0.301</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>-</td>
<td>0.301</td>
</tr>
<tr>
<td>$\Theta_r$</td>
<td>-</td>
<td>0.095</td>
</tr>
<tr>
<td>$\alpha_d$</td>
<td>cm(^{-1})</td>
<td>0.0302</td>
</tr>
<tr>
<td>$\alpha_r$</td>
<td>cm(^{-1})</td>
<td>0.0547</td>
</tr>
<tr>
<td>$\beta_d$</td>
<td>-</td>
<td>8.904</td>
</tr>
<tr>
<td>$\beta_r$</td>
<td>-</td>
<td>4.264</td>
</tr>
</tbody>
</table>
Figure 4.3 Comparison of measured (datapoints) and simulated water content profiles for Dune sand hysteretic flow experiment (Measured data from Gillham et al., 1979).
4.3 Cation Transport and Exchange

The following test problem involves reactive solute transport under steady state flow conditions. Two cases are considered. Both involve transport of cations with retardation due to cation exchange. The first case considers simultaneous transport of calcium and magnesium through Yolo loam soil. Data for this case have been taken from an experiment described by Lai and Jurinak (1972). A 25 cm long column was initially saturated with a 125 mM CaCl₂ solution. At the start of the experiment, the CaCl₂ solution was replaced by a solution containing 62.5 mM of MgCl₂ and 62.5 mM of CaCl₂. The displacing solution was applied for a period of 3.9 hr. Subsequently, the injected solution was switched back to the original CaCl₂ solution. A constant hydraulic flux of 2.64 cm/hr was maintained throughout the experiment. HYDRUS is used to simulate the Mg breakthrough curve. The effect of cation exchange on Mg transport could in this case be described using a linear isotherm with a partition coefficient of $k_d = 0.85 \text{ cm}^2/\text{gr}$. The parameters describing Mg transport are summarized in Table 4.5.

A comparison of the observed and HYDRUS simulated Mg breakthrough curve is presented in Figure 4.4. The observed data are represented by the datapoints while the HYDRUS result is shown as the solid line. It can be seen that the simulated breakthrough curve compares very closely with the observed data. As a further verification of the HYDRUS transport solution, the analytical solution (see van Genuchten and Parker, 1984) of the Mg transport problem is also shown in Figure 4.4 (dashed line). Agreement between the numerical HYDRUS solution and the analytical solution is also excellent.

The second case considered also involves transport with cation exchange between calcium and magnesium. The experiment modeled...
in case 2 was conducted by Selim et al., 1987. The soil in this experiment was Abist loam. The experiment was conducted in a similar way as the experiment of Lai and Jurinak (1972), described above. A 10.75 cm long soil column was first saturated with a 10 meq/L CaCl₂ solution. The experiment consisted of applying a 14.26 pore volume pulse of 10 meq/L MgCl₂ solution, followed by the original CaCl₂ solution. The measured magnesium breakthrough curve again provides the data to verify the HYDRUS transport solution. The difference with the previous case is that for the Abist loam used in the experiment of Selim et al. (1987), the Mg exchange isotherm is nonlinear. The isotherm was determined by Selim et al. using batch experiments and is shown in Figure 4.5. In order to simulate the Mg transport problem with HYDRUS, the Freundlich isotherm (Eq 24a) was fitted to the isotherm data shown in Figure 4.5. The best-fit isotherm is shown as the solid line in Figure 4.5. The corresponding Freundlich isotherm parameters, as well as the other transport parameters for this problem are listed in Table 4.6. The observed Mg breakthrough curve is shown in Figure 4.6, together with the simulated breakthrough curve obtained with HYDRUS. It can be seen that the predicted breakthrough curve describes the measured data reasonably well, but agreement is less good than was obtained in the previous case. Part of the discrepancies between the observed and simulated breakthrough curve may be due to the fact that the batch isotherm measurements do not exactly represent the isotherm for the flowing column system. The observed data in Figure 4.6 also exhibit considerable scatter which may indicate a lack of accurate experimental data.
Table 4.5 Parameters for Mg transport in Yolo loam (after Lai and Jurinak, 1972)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column length, L</td>
<td>cm</td>
<td>25.0</td>
</tr>
<tr>
<td>Pulse duration, $t_o$</td>
<td>hr</td>
<td>3.9</td>
</tr>
<tr>
<td>Water content, $\theta$</td>
<td></td>
<td>0.448</td>
</tr>
<tr>
<td>Bulk density, $\rho_b$</td>
<td>g/cm$^3$</td>
<td>1.32</td>
</tr>
<tr>
<td>Flow rate, q</td>
<td>cm/hr</td>
<td>2.64</td>
</tr>
<tr>
<td>Source concentration, $c_o$</td>
<td>mM</td>
<td>62.5</td>
</tr>
<tr>
<td>Dispersion coefficient, $D$</td>
<td>cm$^2$/hr</td>
<td>0.696</td>
</tr>
<tr>
<td>Partition coefficient, $k_d$</td>
<td>cm$^2$/gr</td>
<td>0.85</td>
</tr>
<tr>
<td>Retardation factor, $R$</td>
<td></td>
<td>3.504</td>
</tr>
</tbody>
</table>
Figure 4.4 Mg breakthrough curve for Ca - Mg transport in Yolo loam with linear isotherm. Observed data from Lai and Jurinak (1972)
Table 4.6 Transport parameters for Mg transport in Abist loam (Selim et al., 1987)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column length, L</td>
<td>cm</td>
<td>10.75</td>
</tr>
<tr>
<td>Pulse duration, $t_o$</td>
<td>hr</td>
<td>358.05</td>
</tr>
<tr>
<td>Water content, $\theta$</td>
<td></td>
<td>0.633</td>
</tr>
<tr>
<td>Bulk density, $\rho_b$</td>
<td>gr/cm³</td>
<td>0.884</td>
</tr>
<tr>
<td>Flow rate, $q$</td>
<td>cm/hr</td>
<td>0.271</td>
</tr>
<tr>
<td>Source concentration, $c_o$</td>
<td>meq/L</td>
<td>10.0</td>
</tr>
<tr>
<td>Dispersion coefficient</td>
<td>cm²/hr</td>
<td>1.167</td>
</tr>
<tr>
<td>Freundlich coefficient, $k_f$</td>
<td>cm³/gr</td>
<td>1.687</td>
</tr>
<tr>
<td>Freundlich exponent, $\eta$</td>
<td></td>
<td>1.615</td>
</tr>
</tbody>
</table>
Figure 4.5 Mg$^{2+}$ exchange isotherm for Abist loam. Data points from Selim et al. (1987). Solid curve represents fitted Freundlich isotherm.
Figure 4.6 Mg$^2+$ breakthrough curve for Abist loam. Data points represent measured data (Selim et al., 1987); solid curve represents HYDRUS simulation.
5. HYDRUS USER'S GUIDE

5.1 Code Structure and Flow Chart

HYDRUS consists of a main program, eight subroutines and three functions. A list of program units and their operation is given below:

- **MAIN**: Controls program execution and calls program subroutines.
- **DATAIN**: Reads the input data and echoes this data back to the output file.
- **DEFINT**: Determines the initial nodal water content values and, if a hysteretic flow simulation is to be performed, initializes nodal arrays used for hysteris modeling.
- **FLOW**: Solves the variably saturated flow equation for the current timestep. If a transport simulation only is performed, this subroutine is called once at the beginning of the simulation to solve the steady state flow equation.
- **UPDATE**: Updates the nodal water contents and, if a hysteretic simulation is performed, determines whether reversal in the saturation paths for every node have occurred and updates the hysteresis arrays. This subroutine is called following every call to subroutine FLOW.
- **HYPR**: Computer nodal values of hydraulic conductivity, water content and analytic moisture retention derivative during flow equation solution.
- **ROOT**: Computer nodal values of root water uptake rate during flow equation solution.
- **SOLUTE**: Solves the advective - dispersive transport equation for the current time step.
- **WROBS**: Writes values of pressurehead, water content, and/or concentration at specified observation depths at the end of every time step.

5-1
WRITES: Writes nodal values of pressure head, water content, and/or concentration at specified time values.

NEXT: Computes the new timestep value and updates the values of transient boundary conditions for the new time value.

TOTALT: Computes the total amount of water or solute present in the soil profile as part of the mass balance computation. Integration of nodal values is performed using the trapezoidal rule.
Figure 5.1 HYDRUS flow chart

5-3
5.2 Data Input Instructions

Data input for HYDRUS is specified in 12 groups, arranged as follows:

Group 1. Problem Description
2. Control Parameters
3. Problem Specification Parameters
4. Time Stepping Parameters
5. Problem Geometry
6. Soil Hydraulic Properties
7. Solute Transport Properties
8. Root Uptake Parameters
9. Initial Conditions
10. Boundary Conditions
11. Output times
12. Observation Point Locations

The input data are read from a formatted file, connected to file unit 5. The user is prompted for the name of the input file at run time. An explanation of each input group is given in the following section. Input formats are described in Section 5.2.2. Example input files and output files are shown in Section 6.
5.2.1 Description of Data Input Groups

Group 1: Problem Description
The first two lines of the data file are reserved to give a descriptive title for the problem. This information is echoed to the output file.

Group 2: Control Parameters
This group contains integer parameters that control program operation, i.e., the type of simulation that is to be performed. The first parameter in this group, ITKOD, controls whether a flow or transport simulation, or both, are performed. When a transport simulation is selected (ITKOD = 1), HYDRUS first solves the steady state flow equation for the specified boundary conditions, from which it obtains the water content distribution and velocity field, followed by the transient transport simulation. To ensure convergence of the steady state flow equation, the specified initial pressure head distribution should approximate the steady state distribution. The third parameter, ICOKOD, controls the type of surface concentration boundary condition to be used for a transport simulation. If ICOKOD = 0, a third type boundary condition is used. This corresponds to specifying the solute concentration of the infiltrating water. If ICOKOD = 1, a first type boundary condition is used. This corresponds to specifying the actual solute concentration at the soil surface. Upstream weighting of the flow solution (IUFPKOD = 1) can be used to improve convergence for certain highly nonlinear flow problems. Two options are available for mass lumping of the storage matrix in the flow equation. The first, ILKOD = 0, corresponds to the use of Eq (35), the L1-scheme. Alternatively, mass lumping according to Eq (36) (L2-Lumping) is used when ILKOD = 1. In either case, the soil moisture capacity values are computed as outlined in Section 3.1.1. to assure a mass-conservative solution. Parameter ICPKOD specifies how the_
initial condition for flow simulation is specified. If ICFKOD = 0, the initial condition is given in terms of pressure head. If ICFKOD = 1, the initial condition is specified in terms of water content. In this case, the code will convert the initial water contents to pressure heads. Note that this option can only be used for a non-hysteretic flow simulation (IHKOD = 0). When a hysteretic flow simulation (IHKOD = 1) is desired, both initial water contents and pressure heads are required. Parameter IBCKOD specifies how boundary conditions change with time. If IBCKOD=0, the boundary conditions are constant in time except for stepwise changes at specified time values (see input group 10). In this case, the time variation of boundary conditions can be represented as a bar graph. If IBCKOD = 1, boundary conditions are interpolated linearly in time between the values specified in input group 10. In this case, the time variation of boundary conditions can be represented as a piece-wise linear function.

If the output from HYDRUS is to be plotted, the output code, IOKOD, should be set to 1, 2, or 3. In this case the requested output is written to plot output files connected to units 7 and 8, respectively. The output in these files is written in a x,y,z column format which facilitates interfacing with most plotting and graphing packages.

If the restart code, IRSKOD, is set equal to 1, the computed nodal values of pressure head, water content and/or concentration at the final time step will be written to the output file. These values can be edited to provide initial conditions for a subsequent simulation.
Group 3: Problem Specification Parameters

This group contains parameters specifying the problem to be simulated. Note the following upper dimensioning limits:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>NMAT</td>
<td>5</td>
</tr>
<tr>
<td>NLAYR</td>
<td>20</td>
</tr>
<tr>
<td>NBC</td>
<td>50</td>
</tr>
<tr>
<td>NPRINT</td>
<td>50</td>
</tr>
<tr>
<td>NOBS</td>
<td>10</td>
</tr>
</tbody>
</table>

NSTEPS is a user-set value for the maximum number of time steps to be allowed. This parameter serves as a guard against excessively long execution time and is particularly useful when a flow simulation shows very slow convergence.

Group 4: Time Stepping Parameters

This group contains time stepping parameters, and the relative and absolute pressure head convergence tolerance, TOL1 and TOL2, respectively, for the iterative flow simulation. The final parameter in this group, CTOL, represents the concentration convergence tolerance for a transport simulation with nonlinear isotherms. It is recommended to use a small value for the starting time step (DELIN), especially for very nonlinear problems, e.g., infiltration into very dry soil. The code will adjust the time step size automatically, depending on the number of iterations required for convergence of the nonlinear flow solution. During a transport run HYDROS automatically ensures that the Courant number does not exceed 1. The time step size is also not allowed to exceed DELMAX. The simulation stops when either time TMAX is reached or the number of time steps exceeds NSTEPS. Parameter NITMAX controls the maximum number of allowable iterations per timestep. If the number of iterations exceeds NITMAX and the flow solution has not reached convergence, the timestep is reduced by half. The default and recommended value is NITMAX = 10. A larger value, e.g., NITMAX = 25 should be used for steady state flow problems (ITKOD = 1).

5-7
Group 5: Problem Geometry
In this group the material type (MAT) and depth of each layer in the soil profile, as well as the nodal spacing for each soil layer, are specified. MAT is an integer code, from 1 to NMAT, assigned to each each layer. This code corresponds to a specific set of hydraulic and transport properties which are specified in Groups 6 and 7. Note that HYDRUS uses the convention that the origin is at the soil surface and the z-coordinate increases downward. In the current version of HYDRUS, the nodal spacing is constant within each soil layer, but can be different between layers. To obtain a desired discretization, the user may specify layers with different nodal spacings but identical material properties. For transport simulations, the nodal spacing should not exceed 3 or 4 times the dispersivity. When flow is steady state, the nodal spacing should not exceed 2 times the dispersivity. Finally, the maximum for the total number of elements is 200.

Group 6: Soil Hydraulic Properties
In this group, the parameters in van Genuchten's model for soil hydraulic properties are specified, see eq. (8) and (9). The correspondence with program variable names is as follows:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_s$</td>
<td>SATK</td>
</tr>
<tr>
<td>$\theta_r$</td>
<td>WCR</td>
</tr>
<tr>
<td>$\theta_s$</td>
<td>WCSD</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>AD</td>
</tr>
<tr>
<td>$\beta_d$</td>
<td>BD</td>
</tr>
<tr>
<td>$\theta_w$</td>
<td>WCSW</td>
</tr>
<tr>
<td>$\alpha_w$</td>
<td>AW</td>
</tr>
<tr>
<td>$\beta_w$</td>
<td>BW</td>
</tr>
</tbody>
</table>

5-8
The hydraulic parameters need to be specified for every material in the soil profile, i.e., from 1 to NMAT. The last three parameters in this group are used only for a hysteretic flow simulation (ITKOD = 1, see group 2), otherwise they should be omitted. Note that Group 6 must always be specified in the data input file, even when only a transport simulation is performed (ITKOD = 1, see group 2). In this case, HYDRUS assumes that flow is steady, and the code will use the hydraulic parameters to first compute the steady state flow solution for the given flow boundary conditions (group 10).

Group 7: Solute Transport Parameters
In this group, the solute transport parameters are specified, see eq. (20) - (24). Note: this group must be omitted if the transport simulation is not performed. The correspondence with program variable names is as follows:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>D^0</td>
<td>DIF</td>
</tr>
<tr>
<td>ε</td>
<td>DISP</td>
</tr>
<tr>
<td>p_b</td>
<td>BULKD</td>
</tr>
<tr>
<td>k_1</td>
<td>PCOF</td>
</tr>
<tr>
<td>η</td>
<td>FEXP</td>
</tr>
<tr>
<td>λ_1</td>
<td>DONE</td>
</tr>
<tr>
<td>λ_2</td>
<td>DSONE</td>
</tr>
</tbody>
</table>

The transport parameters must be specified for each material in the soil profile, i.e., from 1 to NMAT.

Group 8: Root Uptake Parameters
In this group the parameters of the root water uptake function (Eqs. 10-12) are specified, together with the root-depth distribution. It is assumed that the root distribution changes with depth in a piece-wise linear fashion, where NRZ is the
number of linear segments with non-zero root density. The user must specify the root density at each of the NIKZ+1 depth values, starting at the top of the root zone and going downward. Note that the code automatically normalizes the root density distribution, if necessary. This group should be omitted if IRUKOD = 0 (see group 2).

Group 9: Initial Conditions

Initial conditions must be specified at least for the soil surface and for the bottom of the profile. The code will use linear interpolation to determine initial conditions at intermediate nodal points. The user can specify the initial condition for arbitrary additional depths in the profile. For a flow simulation without hysteresis, the user can give the initial condition either in terms of pressure head, or in terms of water content (see ICKOD in group 2). For a flow simulation with hysteresis, both pressure heads, water contents and the hysteresis index (KAP) must be specified. KAP should be set to -1 when the soil at the given depth is initially drying, and to +1 when the soil is initially wetting. The default value is -1.

When the water content for a hysteretic simulation is not specified, it will be computed from the pressure head under the assumption the water content corresponds to the main drying curve (when KAP = -1), or the main wetting curve (when KAP = +1).

For a transport simulation the initial concentration must be specified (default is zero initial concentration).

Group 10: Boundary Conditions

In this group the time dependent boundary conditions are specified. If the boundary conditions do not change, only one set of values needs to be given (NRC = 1, group 2). The time value given for BCTIM(1) is the starting time for the simulation.
(usually BCTIM(1) = 0). HYDRUS allows for boundary conditions that either change step-wise (IBCKOD = 0, group 2) or change continuously (IBCKOD = 1, group 2). When continuous change is specified (IBCKOD = 1) the boundary condition values are linearly interpolated in time. The maximum number of boundary condition changes allowed is 50. Note that one set of flow boundary conditions must be given in case the flow is steady state (ITKOD = 1, see group 2).

**Group 11: Output Times**

Output from HYDRUS is written for all time values specified in this group. The maximum number of output time values is 50.

**Group 12: Observation Point Locations**

Up to 10 different observation points can be specified. A time record of the values of pressure head, water content and/or concentration at each observation point is written to file unit 8. If the location of an observation point does not coincide with one of the nodal points, HYDRUS will linearly interpolate between the neighboring nodal values.
5.2.2 Hydrus Data Input Formats

Group 1: PROBLEM DESCRIPTION (2A60)
2 records.
Col. 1-60 TITLE(1) Descriptive title for case
    1-60 TITLE(2)

Group 2: CONTROL PARAMETERS (10I5)
1 record.
Col. 1-5 ITKOD Simulation control code
    = 0 Flow simulation only
    = 1 Transport simulation only (steady flow)
    = 2 Simultaneous flow and transport.

6-10 INKOD Hysteresis code (leave blank if ITKOD = 1)
    = 0 Perform non-hysteretic flow simulation
    = 1 Include hysteresis in flow simulation.

11-15 IKOKOD Concentration boundary condition code (leave blank if ITKOD = 0)
    = 0 Third type at soil surface
    = 1 First type ar soil surface.

16-20 IRUKOD Root water uptake code
    = 0 No root water uptake
    = 1 Include root water uptake in flow modeling.

21-25 IUFPKOD Hydraulic conductivity upstream weighting code (leave blank if ITKOD = 1)
    = 0 Do not use upstream weighting
    = 1 Use full upstream weighting.

5-12
<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>26-30</td>
<td><strong>ILKOD</strong> Mass matrix lumping code for flow (leave blank if ITKOD = 1)</td>
</tr>
<tr>
<td></td>
<td>= 0 Mass-conservative L1 lumping</td>
</tr>
<tr>
<td></td>
<td>= 1 Mass-conservative L2 lumping.</td>
</tr>
<tr>
<td>31-35</td>
<td><strong>ICFKOD</strong> Initial condition code for non-hysteretic flow simulation</td>
</tr>
<tr>
<td></td>
<td>= 0 Initial pressure head is specified</td>
</tr>
<tr>
<td></td>
<td>= 1 Initial water content is specified</td>
</tr>
<tr>
<td>36-40</td>
<td><strong>IBCKOD</strong> Boundary condition code</td>
</tr>
<tr>
<td></td>
<td>= 0 Boundary conditions change step wise at specified times.</td>
</tr>
<tr>
<td></td>
<td>= 1 Boundary conditions change linearly between specified times.</td>
</tr>
<tr>
<td>41-45</td>
<td><strong>IOKOD</strong> Output code</td>
</tr>
<tr>
<td></td>
<td>= 0 Only regular output is written</td>
</tr>
<tr>
<td></td>
<td>= 1 Nodal values of pressure head, water content and concentration are written to unit 7 for plotting</td>
</tr>
<tr>
<td></td>
<td>= 2 Write time record of computed pressure head, water content and/or concentration at observation points to unit 8</td>
</tr>
<tr>
<td></td>
<td>= 3 Combine IOKOD = 1 and IOKOD = 2.</td>
</tr>
<tr>
<td>46-50</td>
<td><strong>IRSKOD</strong> Restart code</td>
</tr>
<tr>
<td></td>
<td>= 0 Values at final time step are not written</td>
</tr>
<tr>
<td></td>
<td>= 1 Nodal values at final time step are written to output file for subsequent restart.</td>
</tr>
</tbody>
</table>
Group 3: PARAMETERS (6I5, F10.0)
1 record.
Col. 1-5 NSTEPS Maximum number of time steps permitted.
6-10 NMAT Number of different soil materials (maximum = 5).
11-15 NLAYR Number of soil layers (maximum = 20).
16-20 NBC Number of boundary condition time values to be read (maximum = 50).
21-25 NPRINT Number of output time values (maximum = 50).
26-30 NOBS Number of observation points (maximum = 10).
31-40 CNN Solute concentration in groundwater (leave blank if ITKOD = 0).

Group 4: TIME STEPPING AND ITERATION PARAMETERS (6F10.0,IF10.0)
1 record.
Col. 1-10 DELIN Initial time step.
11-20 DELMIN Minimum time step.
21-30 DELMAX Maximum time step.
31-40 TMAX Maximum simulation time.
41-50 TOL1 Relative pressure head convergence tolerance.
51-60 TOL2 Absolute pressure head convergence tolerance.
61-65 NITMAX Number of iterations per time step before time step size is reduced.
66-75     CTOL     Concentration convergence criterion (Used only with nonlinear sorption).

Group 5: PROBLEM GEOMETRY (215,2F10.0)
No. of records = NLAYR (IL = 1 to NLAYR)

<table>
<thead>
<tr>
<th>Col.</th>
<th>1-5</th>
<th>IL</th>
<th>Soil Layer number</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-10</td>
<td>MATL(IL)</td>
<td>Material number for layer IL.</td>
<td></td>
</tr>
<tr>
<td>11-20</td>
<td>TOPL(IL)</td>
<td>Top of layer (from soil surface).</td>
<td></td>
</tr>
<tr>
<td>21-30</td>
<td>BOTL(IL)</td>
<td>Bottom of layer (from soil surface).</td>
<td></td>
</tr>
<tr>
<td>31-40</td>
<td>DELZ(IL)</td>
<td>Nodal spacing to be used in discretizing layer.</td>
<td></td>
</tr>
</tbody>
</table>

Group 6: SOIL HYDRAULIC PROPERTIES
No. of records = NMAT or NMAT x 2 (for hysteretic simulation) (I = 1 to NMAT).

(a) (5F10.0)

<table>
<thead>
<tr>
<th>Col.</th>
<th>1-10</th>
<th>AD(I)</th>
<th>Retention parameter φ for main desorption θ(h) curve of i-th material.</th>
</tr>
</thead>
<tbody>
<tr>
<td>11-20</td>
<td>BD(I)</td>
<td>Retention parameter φ for main desorption θ(h) curve.</td>
<td></td>
</tr>
<tr>
<td>21-30</td>
<td>WCSD(I)</td>
<td>Saturated water content.</td>
<td></td>
</tr>
<tr>
<td>31-40</td>
<td>WCR(I)</td>
<td>Residual water content.</td>
<td></td>
</tr>
<tr>
<td>41-50</td>
<td>SATK(I)</td>
<td>Saturated conductivity.</td>
<td></td>
</tr>
</tbody>
</table>

(b) (3F10.0) ** Omit if IHKOD = 0 **

<table>
<thead>
<tr>
<th>Col.</th>
<th>1-10</th>
<th>AW(I)</th>
<th>Retention parameter φ for main wetting θ(h) curve of i-th material.</th>
</tr>
</thead>
<tbody>
<tr>
<td>11-20</td>
<td>BW(I)</td>
<td>Retention parameter φ for main wetting θ(h) curve.</td>
<td></td>
</tr>
</tbody>
</table>

5-15
Group 7: SOLUTE TRANSPORT PARAMETERS (7F10.0)

** Omit if ITKOD = 0 **

No. of records is NMAT (I = 1 to NMAT).

Col. 1-10 DIF(I) Apparent molecular diffusion coefficient of I-th material.
11-20 DISP(I) Dispersivity.
21-30 RHO(T) Bulk density.
31-40 DONE(I) Decay coefficient for dissolved phase.
41-50 DSONE(I) Decay coefficient for adsorbed phase.
51-60 FCOP(I) Leading Freundlich isotherm coefficient.
61-70 FEXP(I) Freundlich isotherm exponent; set FEXP = 1.0 for linear isotherm.

Group 8: ROOT UPTAKE PARAMETERS

** Omit if IRUKOD = 0 **

(a) Control parameters (I5,3F10.0)

Col. 1-5 NR2 Number of segments in piecewise linear approximation of root distribution function (maximum = 10).
6-15 APAR1 First parameter \( a_1 \) in root uptake function.
16-25 APAR3 Second parameter \( h_{50} \) in root uptake function.
(b) Root depth distribution \((2F10.0)\)

No. of records is \(NRZ + 1\), for \(IR = 1\) to \(NRZ+1\)

<table>
<thead>
<tr>
<th>Col.</th>
<th>1-10</th>
<th>RZDEP(IR)</th>
<th>Depth value.</th>
</tr>
</thead>
<tbody>
<tr>
<td>11-20</td>
<td>RDEN(IR)</td>
<td>Root density/effectiveness value.</td>
<td></td>
</tr>
</tbody>
</table>

N.B. Start at the tip of the root zone, usually at \(z=0\), and proceed downward.

**Group 9: INITIAL CONDITIONS \((4F10.0, I5)\)**

No. of records is at least 2.

<table>
<thead>
<tr>
<th>Col.</th>
<th>1-10</th>
<th>DPIN</th>
<th>Depth for which initial conditions are specified.</th>
</tr>
</thead>
<tbody>
<tr>
<td>11-20</td>
<td></td>
<td>PI</td>
<td>Pressure head at (z = DPIN).</td>
</tr>
<tr>
<td>21-30</td>
<td></td>
<td>WI</td>
<td>Water content at (z = DPIN).</td>
</tr>
<tr>
<td>31-40</td>
<td></td>
<td>CI</td>
<td>Solute concentration at (z = DPIN) (leave blank if ITKOD = 0).</td>
</tr>
</tbody>
</table>
| 41-45|       | KAP  | Hysteresis index \(\alpha\) at \(z = DPIN\),  
\(= -1\) for drying,  
\(= 1\) for wetting,  
(leave blank if THKOD = 0). |

**Group 10: BOUNDARY CONDITIONS \((F10.0, 2I5, 9F10.0)\)**

No. of records is NBC \((IT = 1\) to NBC).

<table>
<thead>
<tr>
<th>Col.</th>
<th>1-10</th>
<th>BCTIM(IT)</th>
<th>Time value. (Note: the simulation starts at BCTIM(1).)</th>
</tr>
</thead>
</table>
| 11-15|        | IRTYP(IT) | Surface boundary condition for flow at time BCTIM(IT),  
\(= 0\) if pressure head is specified, |

5-17
= 1 if flow rate is specified,
= 2 if total amount of applied water is specified.

16-20 IDRTYP(IT) Lower boundary condition for flow,
= 0 if pressure head is specified,
= 1 if flow rate is specified,
= 2 if pressure gradient is zero (free draining profile).

21-30 BCN1(IT) Value of surface boundary condition.

31-40 BCNN(IT) Value of lower boundary condition (leave blank if IDRTYP(IT) = 2).

41-50 CN1(IT) Concentration of infiltration water (leave blank if ITKOD = 0).

51-60 POTET(IT) Potential evapotranspiration rate (leave blank if IRUKOD = 0).

Group 11: OUTPUT TIME VALUES (7F10.0)
No. of records is NPRINT/7 + 0 or 1.

Col. 1-10 TIMEP(1) Time values for which output is desired.
11-20 . .
51-70 TIMEP(NPRINT)

5-18
** Group 12: OBSERVATION POINT LOCATIONS **

** Omit if IOKOD ≤ 1 **

(a) One record (15)

<table>
<thead>
<tr>
<th>Col.</th>
<th>NOBS:</th>
<th>Number of observation points (maximum = 10).</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(b) No. of records is 1 or 2 (7F10.0)

<table>
<thead>
<tr>
<th>Col.</th>
<th>ZOBS(1)</th>
<th>Location of i-th observation point, for i = 1 to NOBS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11-20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>61-70</td>
<td>ZOBS(NOBS)</td>
<td></td>
</tr>
</tbody>
</table>

5-19
5.3 HYDRUS PROGRAM OUTPUT

HYDRUS uses two output files. The main output file is connected to unit 6 and is used to echo the input data read in, followed by simulation results at the requested output time values. Examples of unit 6 output files are shown in Section 6. The second output file, connected to unit 7, is used to write nodal values of pressure head, water content, and concentration at the requested output times for use in plotting simulation results. This file is written only when the output control parameter IOKOD (group 2) is set equal to 1. The program prompts for the output filename(s) at run time. If the main output file (unit 6) already exists, it will not be overwritten. Instead, program execution will be aborted. The plot output file (unit 7), if already existing, will be overwritten by HYDRUS.

For each requested time value, the main output file (unit 6) contains the nodal coordinates (Depth), nodal pressure heads (P), nodal water contents (WC) and nodal concentrations (C). For a hysteretic simulation, the nodal values of the hysteresis index κ (KAPPA) are also written, indicating which nodes are wetting (KAPPA = 1) and drying (KAPPA = -1). Additionally, the values of a number of the program variables at the last timestep are also written out. These variables are:

- **ISTEP**: Time step number
- **DELT**: Time step value
- **RELAXF**: Pressure head under-relaxation factor
- **RAIN**: Darcy water flow rate at the upper soil boundary; positive for downward flow and negative for upward flow.
- **DRAIN**: Darcy flow rate at the lower soil boundary; positive for downward flow and negative for upward flow.
- **PET**: Potential root water uptake rate.

5-20
ACTET: Actual root water uptake rate.
TRAIN: Cumulative water flux at upper soil boundary since start of simulation.
TDRAIN: Cumulative water flux at upper soil boundary since start of simulation.
TRUPTK: Cumulative root water uptake since start of simulation.
STORW: Amount of water present in the soil.
CINF: Concentration of infiltrating water.
SILTIN: Cumulative amount of solute added at upper soil boundary since start of simulation.
SILTOUT: Cumulative amount of solute leached at lower soil boundary since start of simulation.
STORS: Amount of solute present in soil.

The water and solute mass balance errors that are written to the main output file represent the percentage error in the cumulative mass balance.

When variable IOKOD is set to 1 (group 2), an additional output file is created for graphics post-processing. Nodal values of dependent variables are written to this file for every specified output time value. The format of this file is as follows:

<table>
<thead>
<tr>
<th>Column</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>Depth</td>
</tr>
<tr>
<td>11-20</td>
<td>P</td>
</tr>
<tr>
<td>21-30</td>
<td>WC</td>
</tr>
<tr>
<td>31-40</td>
<td>C</td>
</tr>
</tbody>
</table>
6. EXAMPLE INPUT AND OUTPUT FILES

6.1 Infiltration in Bandelier Tuff

The first of the the example input and output files presented in this section correspond to the first problem discussed in section 4.1 and involve infiltration into dry Bandelier Tuff. The HYDRUS data file for this problem is given in Table 6.1; the corresponding HYDRUS output file is shown in Table 6.2. Note that these input and output files correspond to the case where the mass-conservative flow solution is used.

6.2 Input and Output Files for Problem 4.3b

The second set of HYDRUS input and output files correspond to the second transport simulation discussed in section 4.3. This example problem involves transport of Mg$^{2+}$ with a nonlinear Ca-Mg exchange isotherm (Selim et al., 1987). The HYDRUS data input file for this problem is listed in Table 6.3; the corresponding output file is listed in Table 6.4. To simulate this experiment, HYDRUS first solves the steady state flow equation, followed by the transient Mg transport equation. In order to obtain the desired saturated flow solution, the hydraulic conductivity of the column material is simply set equal to the specified flow rate.
Table 6.1  HYDRUS input file for Bandelier Tuff infiltration.

<table>
<thead>
<tr>
<th>Los Alamos caisson exp.: Infiltration (cm, days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L2 C(h); element size = 5.0 cm</td>
</tr>
<tr>
<td>0 0 0 0 0 2 1 0 0 0</td>
</tr>
<tr>
<td>0.001 0.0001 0.5 7.0 1.0 0.010 15</td>
</tr>
<tr>
<td>1 1 0.0 600.0</td>
</tr>
<tr>
<td>0.0143 1.506 0.3308 0.0 25.0</td>
</tr>
<tr>
<td>0.0 0.0 0.10</td>
</tr>
<tr>
<td>600.0 0.0 0.10</td>
</tr>
<tr>
<td>0.0 1 2 20.0</td>
</tr>
<tr>
<td>5.0 1 2 21.06</td>
</tr>
<tr>
<td>2.0 4.0 7.0</td>
</tr>
</tbody>
</table>
Table 6.2 HYDRUS output file for Bandelier Tuff infiltration.

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PROBLEM CONTROL PARAMETERS</strong></td>
<td></td>
</tr>
<tr>
<td>SIMULATION CONTROL CODE</td>
<td>0</td>
</tr>
<tr>
<td>HYSTERESIS MODELING CODE</td>
<td>0</td>
</tr>
<tr>
<td>TRANSPORT BOUNDARY COND. CODE</td>
<td>0</td>
</tr>
<tr>
<td>ROOT WATER UPTAKE CODE</td>
<td>0</td>
</tr>
<tr>
<td>CONDUCTIVITY UPSTREAM WEIGHTING</td>
<td>0</td>
</tr>
<tr>
<td>FLOW MASS MATRIX OPTION</td>
<td>2</td>
</tr>
<tr>
<td>FLOW INITIAL CONDITION CODE</td>
<td>1</td>
</tr>
<tr>
<td>BOUNDARY CONDITION CODE</td>
<td>0</td>
</tr>
<tr>
<td>PLOT OUTPUT CODE</td>
<td>0</td>
</tr>
<tr>
<td>RESTART OUTPUT CODE</td>
<td>0</td>
</tr>
<tr>
<td><strong>TIME STEPPING PARAMETERS</strong></td>
<td></td>
</tr>
<tr>
<td>INITIAL TIMESTEP</td>
<td>0.100E-02</td>
</tr>
<tr>
<td>MINIMUM TIMESTEP</td>
<td>0.100E-03</td>
</tr>
<tr>
<td>MAXIMUM TIMESTEP</td>
<td>0.500</td>
</tr>
<tr>
<td>TOTAL SIMULATION TIME</td>
<td>7.00</td>
</tr>
<tr>
<td>REL. PR. HEAD CONVERGENCE TOLERANCE</td>
<td>1.00</td>
</tr>
<tr>
<td><strong>NUMBER OF NONLINEAR ITERATIONS</strong></td>
<td>15</td>
</tr>
<tr>
<td><strong>PROBLEM SPECIFICATION PARAMETERS</strong></td>
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<td>NUMBER OF ELEMENTS</td>
<td>120</td>
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<td>MAXIMUM NUMBER OF TIMESTEPS</td>
<td>5000</td>
</tr>
<tr>
<td>NUMBER OF SOIL MATERIALS</td>
<td>1</td>
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<tr>
<td>NUMBER OF SOIL LAYERS</td>
<td>1</td>
</tr>
<tr>
<td>NUMBER OF BOUNDARY COND. TIME VALUES</td>
<td>3</td>
</tr>
<tr>
<td>NUMBER OF BOUNDARY COND. TIME VALUES</td>
<td>2</td>
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<tr>
<td>ELEMENT SIZE</td>
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</tr>
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<td>SOIL DEPTH</td>
<td>0.000</td>
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<tr>
<td>GROUNDWATER SOLUTE CONCENTRATION</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

6-3
PROBLEM GEOMETRY

LAYER NUMBER .......... 1
MATERIAL INDEX ................. (MALT) = 1
LAYER THICKNESS .......... (THICK) = 600,
BEGINNING DEPTH .......... (TOPL) = 0.000E+00
ENDING DEPTH .......... (BOTL) = 600.

SOIL HYDRAULIC PROPERTIES

HYDRAULIC PROPERTIES FOR MATERIAL: 1

<table>
<thead>
<tr>
<th>ALPHA</th>
<th>BETA</th>
<th>WCS</th>
<th>WCR</th>
<th>SAK</th>
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</thead>
<tbody>
<tr>
<td>0.0143</td>
<td>1.5060</td>
<td>0.3308</td>
<td>0.0000</td>
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</table>

BOUNDARY CONDITION DATA

<table>
<thead>
<tr>
<th>TIME</th>
<th>SETYP</th>
<th>CNSTYP</th>
<th>SCMN</th>
<th>CMN</th>
<th>CNSTOT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00E+00</td>
<td>1</td>
<td>2</td>
<td>20.0</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>5.00</td>
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<td>2</td>
<td>21.1</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
</tbody>
</table>

OUTPUT TIME VALUES

| 0.200E+01 | 0.400E+01 | 0.700E+01 |

INITIAL CONDITIONS

<table>
<thead>
<tr>
<th>Depth</th>
<th>P</th>
<th>WC</th>
<th>Depth</th>
<th>P</th>
<th>WC</th>
<th>Depth</th>
<th>P</th>
<th>WC</th>
</tr>
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<tbody>
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6 = 4
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<th>Depth</th>
<th>P</th>
<th>WC</th>
<th>Depth</th>
<th>P</th>
<th>WC</th>
<th>Depth</th>
<th>P</th>
<th>WC</th>
</tr>
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<tbody>
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<td>0.00</td>
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<tr>
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<td>1.04E+00</td>
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<td>35.00</td>
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</tr>
<tr>
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**TIME = 6.000E+00** ******

**MASS BALANCE ERROR (%) WATER:** 0.795

6-6
### Mass Balance Error (G)

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**TIME USED = 642.688 SECONDS**

**TIME LIMIT = 1000 SECONDS**
Table 6.3 HYDRUS input file for Mg transport in Abist Loam.

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Table 6.4 HYDRUS output file for Mg transport in Abist Loam.

```
******* ONE-DIMENSIONAL FLOW AND TRANSPORT MODEL *******
HYDRUS v. 3.2

DATA INPUT FILE: selim.dat

SELM ET AL'S Mg-Ca EXCHANGE PROBLEM (STFIT PAPER)
CM, DAYS, Meq,gr FLUX CONC - Mg BREAKTHROUGH -

*************** PROBLEM CONTROL PARAMETERS *******************
SIMULATION CONTROL CODE ................. (ITCODE) = 1
HYSTERESIS MODELING CODE ............... (ITCODE) = 0
TRANSPORT BOUNDARY COND. CODE ........ (ITCODE) = 1
ROOT WATER UPTAKE CODE ................ (ITRCODE) = 0
CONDUCTIVITY UPSTREAM WEIGHTING ....... (ITUPCODE) = 0
FLUX MASS MATRIX OPTION ............... (ITLMODE) = 0
FLUX INITIAL CONDITION CODE .......... (ITICODE) = 0
BOUNDARY CONDITION CODE .............. (ITBCODE) = 0
PLOT OUTPUT CODE ...................... (ITPCODE) = 0
RESTART OUTPUT CODE ................. (ITRSCODE) = 0

*************** TIME STEPPING PARAMETERS *********************
INITIAL Timestep ...................... (DELMIN) = 0.100E+01
MAXIMUM Timestep ...................... (DELMAX) = 0.2000E+02
TOTAL SIMULATION TIME ............... (TMAX) = 25.0
REL. PR. HEAD CONVERGENCE TOLERANCE ... (CTOL1) = 1.00E+00
ABS. ........... (CTOL2) = 0.0000E+00
NUMBER OF NONLINEAR ITERATIONS ...... (NITMAX) = 25
CONCENTRATION CONVERGENCE TOLERANCE .... (CTOL) = 0.100E-05

*************** PROBLEM SPECIFICATION PARAMETERS *************
MAXIMUM NUMBER OF Timesteps .......... (KSTEPS) = 5000
NUMBER OF SOIL MATERIALS .......... (NUMAT) = 1
NUMBER OF SOIL LAYERS ............... (NLAYR) = 1
NUMBER OF BOUNDARY COND. TIME VALUES .. (NBC) = 2
NUMBER OF OUTPUT TIME VALUES ...... (NPRINT) = 2
NUMBER OF OBSERVATION POINTS ...... (NROBS) = 1
SOIL DEPTH .......................... (TDPTH) = 15.0
GROUNDWATER SOLUTE CONCENTRATION .... (CONC) = 0.0000E+00

6-9
```
PROBLEM GEOMETRY

----------------------------------------
LAYER NUMBER ............ 1
MATERIAL INDEX ................. (MATL) = 1
LAYER THICKNESS ............... (THICK) = 15.0
BEGINNING DEPTH ............... (TOPL) = 0.0000E+00
ENDING DEPTH ................. (BOTL) = 15.0
KINEM SPACING ................. (HELZ) = 0.500

SOIL HYDRAULIC AND TRANSPORT PROPERTIES

----------------------------------------
HYDRAULIC PROPERTIES FOR MATERIAL: 1
ALPHA  BETA  WCS  WCR  SATK
0.0100  2.0000  0.6330  0.2000  6.496E+00

TRANSPORT PROPERTIES FOR MATERIAL: 1
DIF  DISP  RHO  DOME  DSNONE  PDCF  FEXP
0.0000  2.7270  0.8040  0.0000  0.0000  1.6670  1.6151

MAXIMUM VALUE OF GRID PECLET NUMBER IS 0.183 FOR LAYER NO. 1

BOUNDARY CONDITION DATA

----------------------------------------
TIME  INTYP  INYTP  BSW  BCW  CHN  CN1  POTET
0.000  0  0  0.000  0.000  0.000  10.000  0.000
14.920  0  0  0.000  0.000  0.000  0.000  0.000

OUTPUT TIME VALUES

----------------------------------------
0.100E+02  0.150E+02

OBSERVATION POINT COORDINATES

----------------------------------------
10.750

INITIAL CONDITIONS

----------------------------------------

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2.00  0.000E+00  0.6330  0.000E+00  2.50  0.000E+00  0.6330  0.000E+00
3.00  0.000E+00  0.6330  0.000E+00  3.50  0.000E+00  0.6330  0.000E+00
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**INITIAL MOISTURE IN PROFILE:** 9.495D
**INITIAL SALT IN PROFILE:** 0.000D

*STEADY STATE FLOW SOLUTION PERFORMED IN 1 ITERATIONS*

**TIME** = 1.000D

**ISTEP** = 1001  **RAIN** = 6.494E+00  **TRAIN** = 6.494E+00  **CIN** = 1.000D

**DELT** = 1.000E-02  **DRAIN** = 6.494E+00  **TDRAIN** = 6.494E+00  **SLTN** = 8.132E+02

**NIT** = 1  **PET** = 0.000E+00  **TRUEK** = 0.000E+00  **SIK** = 1.762E+00

**RELAX** = 1.000  **ACTET** = 0.000E+00  **STOR** = 0.000E+00  **STORS** = 6.637E+02

**MASS BALANCE ERROR** (% WATER): 0.000

**...**  **SOLUTE**: -0.113

**TIME** = 1.500D

**ISTEP** = 1500  **RAIN** = 6.494E+00  **TRAIN** = 9.734E+00  **CIN** = 0.000E+00

**DELT** = 1.000E-02  **DRAIN** = 6.494E+00  **TDRAIN** = 9.734E+00  **SLTN** = 1.102E+03

**NIT** = 1  **PET** = 0.000E+00  **TRUEK** = 0.000E+00  **SIK** = 3.447E-02

**RELAX** = 1.000  **ACTET** = 0.000E+00  **STOR** = 0.000E+00  **STORS** = 7.602E+02

**MASS BALANCE ERROR** (% WATER): 0.000

**...**  **SOLUTE**: -0.345

**TIME** = 1.500D

**ISTEP** = 1500  **RAIN** = 6.494E+00  **TRAIN** = 9.734E+00  **CIN** = 0.000E+00

**DELT** = 1.000E-02  **DRAIN** = 6.494E+00  **TDRAIN** = 9.734E+00  **SLTN** = 1.102E+03

**NIT** = 1  **PET** = 0.000E+00  **TRUEK** = 0.000E+00  **SIK** = 3.447E-02

**RELAX** = 1.000  **ACTET** = 0.000E+00  **STOR** = 0.000E+00  **STORS** = 7.602E+02

**MASS BALANCE ERROR** (% WATER): 0.000

**...**  **SOLUTE**: -0.345

**TIME** = 1.500D

**ISTEP** = 1500  **RAIN** = 6.494E+00  **TRAIN** = 9.734E+00  **CIN** = 0.000E+00

**DELT** = 1.000E-02  **DRAIN** = 6.494E+00  **TDRAIN** = 9.734E+00  **SLTN** = 1.102E+03

**NIT** = 1  **PET** = 0.000E+00  **TRUEK** = 0.000E+00  **SIK** = 3.447E-02

**RELAX** = 1.000  **ACTET** = 0.000E+00  **STOR** = 0.000E+00  **STORS** = 7.602E+02

**MASS BALANCE ERROR** (% WATER): 0.000

**...**  **SOLUTE**: -0.345

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****** NORMAL TERMINATION TIME = 25.0000 AND STEP NUMBER = 2500 ******
7 REFERENCES


APPENDIX

HYDRUS CODE LISTING

7-1
HYDRUS version 3.2

Allows variable nodal spacing
September 1989

ONE-DIMENSIONAL VARIABLY SATURATED FLOW AND TRANSPORT,
INCLUDING Hysteresis, Root Water Uptake and
NONLINEAR Sorption

DEVELOPED BY

J. B. KOOL

HYDRUS IS A MODIFICATION OF THE PROGRAM
‘WORM’ DEVELOPED BY M. TH. VAN GENUTCHEN
AT THE USDA-ARS SALINITY LABORATORY

IMPLICIT REAL*8 (A-H,O-Z)
CHARACTER*40 FILIN*40,FILOUT*40

LOGICAL LINEAR
COMMON/STOR/ T(201),Y(201),DUMMY(1005)
COMMON/VALNOD/MAT(201),KAPPA(201),P(201),FE(201),WE(201),
 + C(201),CE(201),WSS(201),WRR(201),Z(201),Z2(200) +
COMMON/GPTWO/ITKOD,IKHOD,ICOKD,IKRD,KIOD,ILKOD,ICTKOD,IKCKD,
 + IKIOD,IRSKK
COMMON/GPTH/HE,HN,NSTEPS,MTMAT,MLAYR,MBK,PINT,CMN,TDEP
COMMON/GFORS/DELT,DELMIN,DELMAX,TMAX,NOIL,NOIL2,NLMAX
 + WCSW(5)
COMMON/GPSY/DIS(5),RCHOF(5),RFNP(5),DNE(5),DSWDEF(5)
COMMON/GPERS/NE2,APR1,APR2,APR3,RNDOD(201)
COMMON/GPECN/BCNP(51),IRTP(51),IDRTYP(51),BCNP(51),BCNN(51),
 + CN1(51),POTET(51)
COMMON/GPELV/TIMEP(51)
COMMON/GPWFL/NOB,20BS(10),JOBS(10),FOS(10)
COMMON/UNIT/UNITM,KIN,KOUT,KPRINT,KOBS
DATA SMALL/1.0E-10/

----- DISPLAY OPENING SCREEN -----
WRITE(*,*),
WRITE(*,*),

----- END OF PROGRAM -----
WRITE(*,*) ' HYDRUS version 3.2
WRITE(*,*) ' ONE-DIMENSIONAL, VARIABLY SATURATED
WRITE(*,*) ' FLOW AND TRANSPORT MODEL
WRITE(*,*) ' WITH
WRITE(*,*) ' HYSTERESIS AND ROOT WATER UPTAKE
WRITE(*,*)
---------------------------------------------

-------- OPEN FILES --------
WRITE(*,'(A)') ' ENTER INPUTFILE NAME ---> '
READ(*,'(A)') FILIN
WRITE(*,'(A)') ' ENTER OUTPUTFILE NAME ---> '
READ(*,'(A)') FILOUT
--------
OPEN(KIN,FILE=FILIN,STATUS='OLD')
OPEN(KOUT,FILE=FILOUT,STATUS='NEW')
--------
READ INPUT DATA --------
CALL DATAIN(FILIN,LINER)
-------- INITIALIZE FOR FLOW --------
CALL DEFIN(IHKD,ICKD)
-------- WRITE INITIAL CONDITIONS --------
WRITE(KOUT,1010)
SUMT=BCTIM(1)
-------- COMPUTE TOTAL SOLUTE MASS IN SOIL --------
DO 20 I=1,NN
  MT=MAT(I)
  IF(LINEAR) THEN
    Y(I)=C(I)*(WC(I)+RFCOF(MT))
  ELSE
    Y(I)=WC(I)*C(I)+RFCOF(MT)*C(I)**PEXP(MT)
  ENDF
20 CONTINUE
CALL WRITES(SUMT)
TMNIT=TOTALZ(WC,D2,NN)
TSNIT=TOTALZ(Y,D2,NN)
WRITE(KOUT,1020) TMNIT,TSNIT
-------- INITIALIZE PARAMETERS --------
INew=1
IS=0
IP=1
ISTEP=1
DELN=DELIN
RELAXP=1.0
CUMIN=0.0
TRAIN=0.0
TTRAIN=0.0
TRUPTK=0.0
SLTIN=0.0
SLTOUT=0.0
ERRW=0.0
ERRS=0.0
VMAX=0.0
DLMAXX=DELMAX
IF(INTYP(I).EQ.2) THEN
  PULS=BCN1(I)
  BCN1(I)=0.0
  DLMAXX=MIN(DELMAXX,0.1D0*PULS/SATK(MAT(I)))
ENDIF
DO 26 I=1,NN
  WCE(I)=WC(I)
  PE(I)=P(I)
  CE(I)=C(I)
26 CONTINUE

C

----- SET BOUNDARY CONDITIONS -----  
28 CALL TMEXT(IS,NIT,INew,KRAIN,KDRAIN,DELT,SUMT,VALN1,VALNN,CIN,  
  PET, DLMAXX, VMAX)
  IF(ISTEP.EQ.1.OR.ISTEP.EQ.1) THEN
    CALL UPDATE
  ELSE IF(INTYP(IS).EQ.2.AND.(CUMIN+0.5*RAIN*DELT.GT.0.00001)) THEN
    DLMAXX=DELMAX
    INTYP(IS)=1
    BCN1(IS)=0.0
    KRAIN=1
    VALN=0.0
  ENDIF

C

----- SOLVE FOR FLOW -----  
CALL FLOW(KRAIN,KDRAIN,NIT,ISTEP,VALN1,VALNN,PET,RAIN,DRAIN,ACTET,  
  DELT,SUMT,RELAXF)

C

----- UPDATE NODAL WATER CONTENTS -----  
CALL UPDATE

C

----- CALCULATE TMINF=TOTAL AMOUNT OF WATER IN PROFILE -----  
  TDRAIN=TDRRAIN+DRAIN*DELT
  TRUPTK=TRUPTK+ACTET*DELT
  TMINF=TMINF+TRAIN-TDRAIN-TRUPTK
  IF(INTYP(IS).EQ.2) CUMIN=CUMIN+RAIN*DELT
ENDIF

C

----- CONSTANT FLOW RATE IF ITKOD=1 -----  
IF(ITKOD.EQ.1.AND.ISTEP.GT.1) THEN
  RAIN=RANO
  DRAIN=DRAANO
  TDRAIN=TDRRAIN+DRAIN+DRAIN*DELT
  TRUPTK=TRUPTK+ACTET+DELT
  TMINF=TMINF+TRAIN-TDRAIN-TRUPTK
ENDIF

IF(ITKOD.NE.0) THEN
IF(ISTEP.EQ.1) THEN
    RANO=RAIN
    IF(KRAIN.EQ.1) RANO=BCN1(1)
    DRANO=RAIN
    IF(KDRAIN.EQ.1) DRANO=BCNN(1)
    CINO=CN1(1)
ENDIF

----- SOLVE FOR SOLUTE TRANSPORT ----- 
CALL SOLUTE(RANO, DRANO, RAIN, DRAIN, CINO, CIN, QN1, QNN, DELT, VMAX, * 
    LINEAR)
SLTIN=SLTIN+QN1*DELT
SLTOUT=SLTOUT+QNN*DELT
SMIN=TSINIT+SLTIN-SLTOUT
ENDIF

----- WRITE PRESSURE, MOISTURE AND SOLUTE DISTRIBUTION ----- 
IF(MPRINT.NE.0.AND.SUMT.GE.TIMEP(IP)) THEN
    DELF=(SUMT-TIMEP(IP))/DELT
    DO 70 I=1,NN
        MT=MAT(I)
        T(I)=P(I)
        IF(ITKOD.NE.1) THEN
            P(I)=DELF*P(I)+(1.-DELF)*PE(I)
            WC(I)=DELF*WC(I)+(1.-DELF)*WCE(I)
        ELSE
            P(I)=PE(I)
            WC(I)=WCE(I)
        ENDIF
        IF(ITKOD.NE.0) THEN
            C(I)=DELF*C(I)+(1.-DELF)*CE(I)
            IF(LINEAR) THEN
                Y(I)=CE(I)*(WCE(I)+RFCOF(MT))
            ELSE
                Y(I)=WCE(I)*CE(I)+RFCOF(MT)*CE(I)*FEXP(MT)
            ENDIF
        ENDIF
        Y(I)=WC(I)*CE(I)+RFCOF(MT)*CE(I)*FEXP(MT)
    70 CONTINUE
ENDIF

----- COMPUTE MASS BALANCE ERRORS ----- 
STORM=0.0
STORS=0.0
IF(ITKOD.NE.1.OR.ISTEP.EQ.1) THEN
    STORM=TOTALT(WCE, DZ, NN)
ENDIF
IF(ITKOD.NE.0) THEN
    STORS=TOTALT(V, DZ, NN)
    IF(SMIN.GT.0.0) ERRS=100.0*(SMIN-STORS)/SMIN
ENDIF
IF(ITKOD.EQ.0) THEN
    WRITE(KOUT,1036) TIMEP(IP), ISTEP, RAIN, TRAIN, DELT, DRAIN, 
    TDRAIN, NIT, PET, TRUPPK, RELAX, ACTET, STORM
    WRITE(KOUT,1038) ERRW
    ELSE

C

PURPOSE: TO READ & ECHO INPUT PARAMETERS

SUBROUTINE DATAIN(FILIN, TINFO)

C

IMPLICIT REAL*8 (A-H,O-Z)
CHARACTER TITLE*60, PLTFIL*40, FILIN*40, OBSFIL*40
LOGICAL LINEAR
DIMENSION MATL(20), TOPL(20), BOTL(20), DELZ(20), RZDEP(10), RDEN(10)
COMMON/VAlJOD MAT(201), KAPPA(201), P(201), PE(201), WC(201), WCE(201)
+C(201), CE(201), WSS(201), WR(201), Z(201), DE(200)
COMMON/GPFW/ NKO, NKO, IOKOD, IOKOD, IKCOD, IOKOD, IKCOD, IOKOD, IOKOD
+ IOKOD, IOKOD
COMMON/GPDR/NE, NN, NSTEMPS, NMAT, NLAYR, NBC, NPRINT, CNN, TDEPTH
COMMON/GPFI/DELIN, DELMIN, DELMAX, TMAX, TOL1, TOL2, NMAX
+WCSW(5)
COMMON/GPFD/ NREZ, NPARZ, NPAR2, NPAR3, NORD(201)
COMMON/GPFP/ NBFNT(51), IBTCLF(51), IDRFYP(51), BCN1(51), BCN2(51)
+ CN2(51), PAYET(51)
COMMON/GPFL/ NREZ, NPARZ, NPAR2, NPAR3, NORD(201)
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COMM...
----- GROUP 2: CONTROL PARAMETERS -----

**ITKOD** = TRANSPORT SIMULATION CODE
0: ONLY FLOW
1: ONLY TRANSPORT
2: FLOW + TRANSPORT

**IHKOD** = HYSTERESIS CODE
0: NO
1: YES

**ICOKOD** = TRANSPORT BOUNDARY CONDITION CODE
0: THIRD TYPE (CONCENTRATION OF INCOMING FLUID SPECIFIED)
1: FIRST TYPE (CONCENTRATION AT SOIL SURFACE SPECIFIED)

**IRUKOD** = ROOT WATER UPTAKE CODE
0: NO
1: YES

**IUPKOD** = UPSTREAM WEIGHTING CODE FOR HYDR. CONDUCTIVITY
0: NO
1: YES

**ILKOD** = LUMPING AND MOISTURE CAPACITY CODE
0: L1 LUMPING WITH MASS-CONSERVATIVE C(h)
1: L2 LUMPING WITH MASS-LUMPING C(h)

**ICKOD** = INITIAL CONDITION CODE FOR NON-HYSTERETIC FLOW
0: PRESSURE HEAD IS GIVEN
1: WATER CONTENT IS GIVEN

**IBCKOD** = BOUNDARY CONDITION CODE
0: STEP-WISE CHANGES
1: CONTINUOUS CHANGES (LINEAR INTERPOLATION IN TIME)

**IKOD** = OUTPUT CODE
0: REGULAR OUTPUT ONLY
1: ADDITIONAL PLOT OUTPUT TO UNIT 7

**IRSKOD** = RESTART CODE
0: IF NO FINAL TIMESTEP OUTPUT
1: WRITE NODAL VALUES AT FINAL TIMESTEP

----- GROUP 3: PROBLEM SPECIFICATION PARAMETERS -----

**NSTEPS** = MAXIMUM NUMBER OF TIME STEPS PERMITTED

**NMAT** = NUMBER OF MATERIALS (MAX=5)

**NLAYR** = NUMBER OF SOIL LAYERS (MAX=20)

**NBC** = NUMBER OF BOUNDARY CONDITION TIME VALUES (MAX=50)

**NPRINT** = NUMBER OF OUTPUT TIME VALUES (MAX=50)
NOBS = NUMBER OF OBSERVATION POINTS (MAX=10)
CNN = SOLUTE CONCENTRATION OF GROUNDWATER

-----
READ(KIN,1005) NSTEPS, NMAT, NLAYR, NBC, NPRINT, NOBS, CNN
NMAT=MIN(NMAT,5)
NLAYR=MIN(NLAYR,20)
NBC=MIN(NBC,50)
NPRINT=MIN(NPRINT,50)
NOBS=MIN(NOBS,10)
IF(NOBS.GT.0) THEN
   WRITE(KTERM,'(A)') ' ENTER FILE NAME FOR OBSERVATION POINT',+
   ' OUTPUT ----> ' READ(KTERM,'(A)') OBSFIL
   OPEN(8,FILE=OBSFIL,STATUS='UNKNOWN')
ENDIF

----- GROUP 4: TIME STEPPING PARAMETERS -----
DELIN = INITIAL TIME STEP
DELMIN = MINIMUM TIME STEP
DELMAX = MAXIMUM TIME STEP
TMAX = SIMULATION DURATION
TOL1 = RELATIVE PRESSURE HEAD CONVERGENCE CRITERION
TOL2 = ABSOLUTE
NITMAX = NUMBER OF NONLINEAR ITERATIONS ALLOWED
CTOL = ABSOLUTE CONCENTRATION CONVERGENCE CRITERION
(USED ONLY WITH NONLINEAR SORPTION)

-----
READ(KIN,1017) DELIN, DELMIN, DELMAX, TMAX, TOL1, TOL2, NITMAX, CTOL
IF(NITMAX.EQ.0) NITMAX=10
IF(NMAX.EQ.1) NITMAX=MAX(NMAX,25)
WRITE(KOUT,1010) DELIN, DELMIN, DELMAX, TMAX, TOL1, TOL2, NITMAX
TOL2=MAX(TOL2,SMALL)
IF(CTOL.GT.1.0E-10) WRITE(KOUT,2010) CTOL

----- GROUP 5: PROBLEM GEOMETRY SPECIFICATION -----
IL = SOIL LAYER NUMBER
MATL = SOIL MATERIAL INDEX
TOPL = TOP OF SOIL LAYER
BOTL = BOTTOM OF SOIL LAYER
DEL2 = MODAL SPACING FOR LAYER

-----
TDEPTH=0.0
DO 10 IL=1,NLAYR
   READ(KIN,1015) IL,MATL(IL),TOPL(IL),BOTL(IL),DEL2(IL)
   IF((IL.GT.NLAYR).OR.(MATL(IL).GT.NMAT).OR.+
   *(TOPL(IL).GT.BOTL(IL))) THEN
      WRITE(KOUT,1014) IL
      STOP
   ENDIF
   TDEPTH=MAX(TDEPTH,BOTL(IL))
10 CONTINUE
WRITE(KOUT,1008) NSTEPS, NMAT, NLAYR, NBC, NPRINT, NOBS, TDEPTH, CNN
WRITE(KOUT,1012)
NE=0
NN=1
Z(1)=0.0
DO 12 I=1,NLAYR
    THICK=BOTL(I)-TOPL(I)
    NEIAY=INT(THICK/DELT(I))+0.5001
    DELT(I)=THICK/NEIAY
    WRITE(KOUT,1016) I,MATL(I),THICK,TOPL(I),BOTL(I),DELT(I)
    NENEW=NE+NEIAY
    J1=J+1
    Z(J1)=Z(J)+DELT(I)
    DZ(J)=DELT(I)
11 CONTINUE
    NE=NENEW
    NN=NENEW+1
    IF(NN.GT.NNMAX) THEN
        WRITE(KOUT,1048) NNMAX
        STOP 'ERROR IN GROUP 5: TOO MANY NODES'
    ENDIF
12 CONTINUE

------ ASSIGN MATERIAL PROPERTIES TO NODES ------
    ILR=1
    ZEND=BOTL(1)
    DO 15 I=1,NN
        MAT(I)=1
        IF(Z(I).GT.ZEND) THEN
            ILR=ILR+1
            ZEND=BOTL(ILR)
        ENDIF
    ENDIF
    MAT(I)=MAT(ILR)
15 CONTINUE

------ GROUP 6: SOIL HYDRAULIC PROPERTIES ------
    IM = SOIL MATERIAL INDEX
    AD = PARAMETER ALPHA FOR MAIN DRYING CURVE
    BD = PARAMETER BETA (N) FOR MAIN DRYING CURVE
    WCSD = SATURATED WATER CONTENT
    WCR = RESIDUAL WATER CONTENT
    SATK = SATURATED HYDRAULIC CONDUCTIVITY
    AW = PARAMETER ALPHA FOR MAIN WETTING CURVE
    BW = PARAMETER BETA (N) FOR MAIN WETTING CURVE
    WCSW = MAXIMUM WATER CONTENT UPON REWETTING

    IF(ITKGD.NE.0) THEN
        WRITE(KOUT,1018)
    ELSE
        WRITE(KOUT,1020)
    ENDIF
10 CONTINUE
    DO 20 I=1,NMAT
        IM=I
20 CONTINUE
WRITE(KOUT,1022) IM
READ(KIN,1007) AD(IM),BD(IM),WCSD(IM),WCR(IM),SATK(IM)
IF(IHOD.EQ.1) THEN
READ(KIN,1007) AM(IM),BW(IM),WCWS(IM)
IF(AM(IM).LT.1.E-10) AM(IM)=AD(IM)
IF(BW(IM).LT.1.E-10) BW(IM)=BD(IM)
IF(WCWS(IM).LT.1.E-10) WCWS(IM)=WCSD(IM)
ENDIF
IF(IHOD.EQ.1) THEN
WRITE(KOUT,1024) IM, AM(IM),BW(IM),WCWS(IM),WCR(IM),SATK(IM),
ENDIF
ELSE
WRITE(KOUT,1026) IM, AM(IM),BW(IM),WCWS(IM),WCR(IM),SATK(IM)
END IF
Crear un nuevo grupo: 7: Parámetros de transporte del soluto

IM = Índice del material de suelo

DIF = Coeficiente de difusión efectivo

DISP = Dispersividad

RHO = Densidad

DONE = Coeficiente de descomposición para fase disuelta

DSONE = Coeficiente de descomposición para fase adsorbida

FCOF = Coeficiente de Freundlich (coeficiente de partición)

FEXP = Coeficiente de Freundlich (1.0 si linear isothermo)

Escribir (KOUT,2028) IM, DIF(IM), DISP(IM), RHO, DONE(IM), DSONE(IM), FCOF, FEXP(IM)

IF(IHOD.NE.0) THEN
DO 25 I=1,NMAT
IM=I
READ(KIN,1007) DIF(IM),DISP(IM),RHO,DONE(IM),DSONE(IM),FCOF,
+ FEXP(IM)
RFCOF(IM)=RHO*FCOF
IF(FEXP(IM).LT.1.E-10) FEXP(IM)=1.0
IF(ABS(FEXP(IM)-1.0).GT.0.05) THEN
LINEAR=.FALSE.
WRITE(KOUT,2028) IM,DIF(IM),DISP(IM),RHO,DONE(IM),DSONE(IM),
+ FCOF,FEXP(IM)
ELSE
WRITE(KOUT,1028) IM,DIF(IM),DISP(IM),RHO,DONE(IM),DSONE(IM),
+ FCOF
ENDIF
25 CONTINUE

Comprobar el número de Peclet para el transporte del sistema

PEMAX=0.0
DO 26 I=1,NLAYR
MT=MATL(I)
PELAY=DELSZ(I)/DISP(MT)
IF(PELAY.GT.PEMAX) THEN
ILAY=I
PEMAX=PELAY
ENDIF
WRITE(KOUT,1050) PEMAX,ILAY
ENDIF

----- GROUP 8: ROOT UPTAKE PARAMETERS ------

NRZ = NUMBER OF SEGMENTS IN ROOT DEPTH DISTRIBUTION
APAR1 = FIRST PARAMETER (a1) IN ROOT UPTAKE FUNCTION
APAR2 = SECOND (h50) ...
APAR3 = THIRD (p) ...

RDEN = DEPTH VALUE AT WHICH ROOT DENSITY IS SPECIFIED
RZDEP = ROOT DENSITY/EFFECTIVENESS AT RZDEP

IF(IRUKOD.EQ.1) THEN
READ(KIN,1009) NRZ,APAR1,APAR2,APAR3
WRITE(KOUT,1010) NRZ,APAR1,APAR2,APAR3
CUMRDN=0.0
NRZ=NRZ+1
DO 20 I=1,NRZ
READ(KIN,1007) RZDEP(I),RDEN(I)
WRITE(KOUT,1012) I,RZDEP(I),RDEN(I)
IF(I.GT.1) THEN
CUMRDN=CUMRDN+0.5*(RZDEP(I)-RZDEP(I-1))*(RDEN(I)+RDEN(I-1))
ENDIF
20 CONTINUE

----- INITIALIZE NODAL VALUES OF NORMALIZED ROOT DENSITY ------
IDP=1
DO 32 I=1,NN
DEP=Z(I)
IF(DEP.LT.RZDEP(1).OR.DEP.GT.RZDEP(NRZ)) THEN
RDNOD(I)=0.0
ELSE
IF(DEP.GE.RZDEP(IDP+1)) IDP=IDP+1
DIST=(DEP-RZDEP(IDP))/(RZDEP(IDP+1)-RZDEP(IDP))
RDNODE=DIST*RDEN(IDP+1)+(1.-DIST)*RDEN(IDP)
RDNOD(I)=RDNODE/CUMRDN
ENDIF
32 CONTINUE

----- GROUP 9: INITIAL CONDITIONS ------

DPIN = DEPTH
PI = INITIAL PRESSURE HEAD
WI = INITIAL MOISTURE CONTENT
CI = INITIAL SOLUTE CONCENTRATION
KAP = HYSTERESIS INDEX

= 1: WETTING
= -1: DRYING

IN=1
NODE=1
READ(KIN,1011) DPIN1,P11,W11,C11,KAP
DO 40 INOD=2,NN
READ(KIN,1011) DPIN2,P12,W12,C12,KAP
IF(DPIN2.GT.(TDEPTH+0.01)) THEN
WRITE(KOUT,1042) DPIN2,TDEPTH
STOP ' ERROR IN GROUP 9; SEE OUTPUT FILE'
ENDIF
DO 33 J=NODE,NN
IF((Z(J)+0.0001).GE.DPIN2) THEN
NODE=J-1
GO TO 34
ENDIF
33 CONTINUE
34 DO 35 I=IN,NODE
DEP=Z(I)
DIST=(DEP-DPIN1)/(DPIN2-DPIN1)
P(I)=DIST*P12+(1.-DIST)*P11
WC(I)=DIST*W12+(1.-DIST)*W11
C(I)=DIST*C12+(1.-DIST)*C11
KAPPA(I)=KAP
35 CONTINUE
IF(NODE.EQ.(NN-1)) THEN
DEP=Z(NN)
DIST=(DEP-DPIN1)/(DPIN2-DPIN1)
P(NN)=DIST*P12+(1.-DIST)*P11
WC(NN)=DIST*W12+(1.-DIST)*W11
C(NN)=DIST*C12+(1.-DIST)*C11
KAPPA(NN)=KAP
ELSE
GO TO 42
ENDIF
40 CONTINUE
42 CONTINUE

----- GROUP 10: BOUNDARY CONDITIONS -----
BCTIM = TIME AT WHICH BOUNDARY CONDITIONS BECOME ACTIVE
N.B. SIMULATION STARTS AT BCTIM(1)
IRTYP = CODE FOR UPPER FLOW BOUNDARY CONDITION
0: 1ST TYPE BC
1: FLUX TYPE BC
2: AMOUNT OF INFILTRATION GIVEN
IDRTYP = CODE FOR LOWER FLOW BOUNDARY CONDITION
0: 1ST TYPE BC
   1: FLUX TYPE BC
   2: FREE DRAINAGE BC (PRESSURE GRADIENT ZERO)
BCN1  = VALUE OF UPPER FLOW BC (F10.0)
BCNN  = VALUE OF LOWER FLOW BC (F10.0)
CN1   = SOLUTE CONCENTRATION OF INFILTRATION WATER
POTET = POTENTIAL EVAPOTRANSPIRATION RATE

----------
WRITE(KOUT,1034)
DO 44 I=1,NBC
READ(KIN,1013) BCTIM(I),IRVTYP(I),IDRTYP(I),BCN1(I),BCNN(I),
   + CN1(I),POTET(I)
WRITE(KOUT,1036) BCTIM(I),IRVTYP(I),IDRTYP(I),BCN1(I),BCNN(I),
   + CN1(I),POTET(I)
44 CONTINUE
IF(ITKND.EQ.1.AND.IDRTYP(I).EQ.2) THEN
   WRITE(KOUT,1046)
   STOP 'ERROR IN GROUP 10; SEE OUTPUT FILE'
ENDIF
BCTIM(NBC+1)=TMAX+DELMAX
IRVTYP(NBC+1)=IRVTYP(NBC)
IDRTYP(NBC+1)=IDRTYP(NBC)
BCN1(NBC+1)=BCN1(NBC)
BCNN(NBC+1)=BCNN(NBC)
CN1(NBC+1)=CN1(NBC)
POTET(NBC+1)=POTET(NBC)

----- GROUP 11: OUTPUT TIME VALUES -----}
TIMEP  = OUTPUT TIME VALUES

-----
IF(NPRINT.GT.0) THEN
   READ(KIN,1007) (TIMEP(I),I=1,NPRINT)
   WRITE(KOUT,1038) (TIMEP(I),I=1,NPRINT)
ENDIF

----- GROUP 12: OBSERVATION POINTS -----}
IF(NOBS.GT.0) THEN
   READ(KIN,1007) (ZOBS(I),I=1,NOBS)
   WRITE(KOUT,1052) (ZOBS(I),I=1,NOBS)
   WRITE(KOUT,1054) (ZOBS(I),I=1,NOBS)
ENDIF

----- DETERMINE NODAL INTERPOLATION FACTOR -----}
DO 50 I=1,NOBS
   DO 48 J=2,NN
      IF(Z(J).GE.ZOBS(I)) THEN
         IOBS(I,1)=J-1
         IOBS(I,2)=J
         ZOBS(I)=(Z(J)-ZOBS(I))/DZ(J-1)
      ENDIF
   GO TO 50
50 CONTINUE
C ---- FORMATS ----

1001 FORMAT(A)
1003 FORMAT(10I5)
1005 FORMAT(6I5,G10.0)
1007 FORMAT(7G10.0)
1009 FORMAT(15,3G10.0)
1011 FORMAT(4G10.0,1I5)
1013 FORMAT(G10.0,2I2,4G10.0)
1015 FORMAT(2I5,3G10.0)
1017 FORMAT(6G10.0,1I5,G10.0)

1000 FORMAT(/'///1X,70(1H*),1X,1H*,68X,1H*/*,2,1H*,14X,  
   'ONE-DIMENSIONAL FLOW AND TRANSPORT MODEL',14X,1H/  
   * 1X,1H*,27X,HYDROUS V. 3.2*,27X,1H*/*,1X,1H*,68X,1H/  
   * 1X,1H*,6X,'DATA INPUT FILE: ',A,5X,1H*/*,1X,1H*,60X,1H*)

1002 FORMAT(1X,1H*,4X,A,40,4X,1H*)
1004 FORMAT(1X,1H*,68X,1H*/*,1X,70(1H*))
1006 FORMAT(/'///10X,'PROBLEM CONTROL PARAMETERS'/10X,26(1H*))//  
   * 10X,'SIMULATION CONTROL CODE' ...............(ITKOD) = 'I5/*  
   * 10X,'HYSTERESIS MODELING CODE' ...............(IHKOD) = 'I5/*  
   * 10X,'TRANSPORT BOUNDARY COND. CODE' ..........(IHKOD) = 'I5/*  
   * 10X,'ROOT WATER UPTAKE CODE' ................(IIKOD) = 'I5/*  
   * 10X,'CONDUCTIVITY UPSTREAM WEIGHTING' ........(IJKOD) = 'I5/*  
   * 10X,'FLOW MASS MATRIX OPTION' ................(IKOD) = 'I5/*  
   * 10X,'FLOW INITIAL CONDITION CODE' .......... ....(IKK0D) = 'I5/*  
   * 10X,'BOUNDARY CONDITION CODE' ...............(IHKKD) = 'I5/*  
   * 10X,'PLOT OUTPUT CODE' ........................(IKOKD) = 'I5/*  
   * 10X,'RESTART OUTPUT CODE' ........................(IKR0D) = 'I5/*

1008 FORMAT(/'///10X,'PROBLEM SPECIFICATION PARAMETERS'/10X,32(1H*))//  
   * 10X,'MAXIMUM NUMBER OF Timesteps' ............(NSTEP) = 'I5/*  
   * 10X,'NUMBER OF SOIL MATERIALS' ..............(NMAT) = 'I5/*  
   * 10X,'NUMBER OF SOIL LAYERS' ..................(NLAY) = 'I5/*  
   * 10X,'NUMBER OF BOUNDARY COND. TIME VALUES' ... (NHTC) = 'I5/*  
   * 10X,'NUMBER OF OUTPUT TIME VALUES' ........... (NPRNT) = 'I5/*  
   * 10X,'NUMBER OF OBSERVATION POINTS' ........... (NOBS) = 'I5/*  
   * 10X,'SOIL DEPTH' ..............................(TDEPTH) = 'G10.3/*  
   * 10X,'GROUNDWATER solute CONCENTRATION' ...... (CWW) = 'G10.3/*

1010 FORMAT(/'///10X,'TIME STEPPING PARAMETERS'/10X,24(1H*))//  
   * 10X,'INITIAL Timestep' .........................(DELIN) = 'G10.3/*  
   * 10X,'MINIMUM Timestep' ........................(DEMIN) = 'G10.3/*  
   * 10X,'MAXIMUM Timestep' ........................(DEMAX) = 'G10.3/*  
   * 10X,'TOTAL SIMULATION TIME' .................(TMAX) = 'G10.3/*  
   * 10X,'REL. PR. HEAD CONVERGENCE TOLERANCE' ......(TOI) = 'G10.3/*  
   * 10X,'LAPS' ................................. ....(TOL2) = 'G10.3/*  
   * 10X,'NUMBER OF NONLINEAR iterations' ..........(NITMAX) = 'I5/*  

2010 FORMAT(10X,'CONCENTRATION CONVERGENCE TOLERANCE' ... (CTOL) = 'G10.3/*

1012 FORMAT(/'///10X,'PROBLEM GEOMETRY'/10X,16(1H*))
1014 FORMAT(/'///5X,'*** ERROR IN INPUT GROUP 5: CHECK LAYER',I3,",I3,",I3,",I3")
1016 FORMAT(/'///10X,'LAYER NUMBER' ...............',I3/
10X,'MATERIAL INDEX'..........................(MATL) = 'I5',
' THICKNESS'..................THICK = '010.3/
' BEGINNING DEPTH'..................(BEGD) = '010.3/
' ENDING DEPTH'..................(ENDD) = '010.3/
' MODAL SPACING'..................(DELS) = '010.3/

1018 FORMAT('I10X,'SOIL HYDRAULIC AND TRANSPORT PROPERTIES'/
 ' 10X,39(1H=))
1020 FORMAT('I10X,'SOIL HYDRAULIC PROPERTIES'/10X,25(1H=))
1022 FORMAT('I10X,'HYDRAULIC PROPERTIES FOR MATERIAL':',I2//'10X,
 ' ALPHA Beta wcs wcr satk '10X,

1024 FORMAT('I10X,
 ' DRYING ',4F8.4,1PE10.3/10X,
 ' WETTING ',3(0F8.4))
1026 FORMAT('I10X,4F8.4,1PE10.3)
1028 FORMAT('I10X,'TRANSPORT PROPERTIES FOR MATERIAL':',I2//'10X,
 ' DIP DISP RHO DONE DSCNE KD'/10X,
 ' ',8X,
 ' 6F8.4)
2028 FORMAT('I10X,'TRANSPORT PROPERTIES FOR MATERIAL':',I2//'10X,
 ' DIP DSCN RHO DONE DSCNE FCNF FEXP'/10X,
 ' ',8X,
 ' 7F8.4)
1030 FORMAT('I10X,'ROOT UPTAKE PARAMETERS'/10X,22(1H=)
 ' NUMBER OF ROOTZONE SEGMENTS'..................(NRZ) = 'I5/
 ' FIRST ROOT UPTAKE PARAMETER (a1) ...............(APR1) = 'G10.3/
 ' SECOND ROOT UPTAKE PARAMETER (h50) ............(APR2) = 'G10.3/
 ' THIRD ROOT UPTAKE PARAMETER (p) ...............(APR3) = 'G10.3/
 ' SEGMENT DEPTH ROOT DENSITY'/10X,37(1-1))
1032 FORMAT('I10X,14,5X,G10.3,7X,G10.3)
1034 FORMAT('I10X,'BOUNDARY CONDITION DATA'/10X,23('=',12X,
 ' TIME
 ' IN
 ' CN1 PCTET')
1036 FORMAT(7X,F10.3,4X,I3,1X,I5,2X,F10.3)
1038 FORMAT('I10X,'OUTPUT TIME VALUES'/10X,19(1='//
 ' 10X,7E10.3)
1040 FORMAT('I10X,'HYSTERESIS OPTION (IHKOD=1) MUST NOT BE USED',
 ' STANDE STATE FLOW OPTION (ITKOD=1)
1042 FORMAT('I10X,'DEPTH ',G10.3,' IS GREATER THAN SPECIFIED SOIL',
 ' DEPTH OF ',G10.3)
1044 FORMAT('I10X,'COMPUTED ',G10.3,' AND SPECIFIED ',G10.3,'',
 ' SOIL DEPTH DO NOT AGREE/
1046 FORMAT('I10X,'PULSE BOUNDARY CONDITION (ITRP=2) MUST NOT BE',
 ' USED WITH STANDE STATE FLOW (ITKOD=1)
1048 FORMAT('I10X,'*** ERROR IN INPUT GROUP 5: NUMBER OF NODES EXCEEDS',
 ' 15, IS, ***)
1050 FORMAT('I10X,'MAXIMUM VALUE OF GRID PECLET NUMBER IS',F8.3,
 ' FOR LAYER NO.',I3)
1052 FORMAT('I10X,'OBSERVATION POINT COORDINATES'/10X,29('=',10X,
 ' 10X,10F10.3)
1054 FORMAT(15X,'OBSERVATION POINT VALUES'/
 ' 5X,' TIME ',10F11.3)

C----------------------------------------
SUBROUTINE DEFRNT(IHKOD,ICKOD)
PURPOSE: TO INITIALIZE WSS AND WRR ARRAYS FOR HYSERETIC SIMULATION

------

IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VALMOD/MAT(201),KAPPA(201),P(201),PE(201),WC(201),WCE(201)
+ .C(201),CE(201),WSS(201),WRR(201),Z(201),ZI(200)
COMMON/GPTHR/N,NE,NN,NSTEPS,NMAT,NLAYR,NBC,NIPRINT,CNH,TDDEPHT
+ WCSW(5)
COMMON/UNITS/XTERM,KIN,KOUT,KPLT,KOBS
DATA ZERO/0.0/,SMALL/1.0E-06/
------

IF(ZHMOD.EQ.0) THEN

----- INITIALIZE FOR NON-HYSERETIC SIMULATION -----
DO 20 I=1,NN
MT=MAT(I)
KAPPA(I)=1.0
WRR(I)=WCR(MT)
WSS(I)=WCSD(MT)
IF(1CKOD.EQ.0) THEN

----- COMPUTE WATER CONTENT FROM PR. HEAD -----
   SED=(1.+(MT)^P(I))*BD(MT)**(1./BD(MT)-1.)
   WC(I)=WRR(I)+(WSS(I)-WRR(I))*SED
ELSE
   WC(I)=WSS(I)
ENDIF
ELSE

----- COMPUTE PR. HEAD FROM WATER CONTENT -----
IF(WC(I).LT.WCSD(MT)) THEN
   RMM=BD(MT)/(1.-BD(MT))
   SED=(WC(I)-WCR(MT))/(WCSD(MT)-WCR(MT))
   P(I)=-(SED**RMM-1.)*(1./BD(MT))/AD(MT)
ELSE
   P(I)=0.0
ENDIF
ENDIF
20 CONTINUE
RETURN
ELSE

----- INITIALIZE FOR HYSERETIC CASE -----
DO 30 I=1,NN
MT=MAT(I)
PR=ABS(P(I))
IF(KAPPA(I).EQ.-1) THEN
   SED=(1.+(MT)**PR)**BD(MT)**(1./BD(MT)-1.)
IF(WC(I).LT.1.0E-10) THEN

----- START FROM DRYING BOUNDARY-----
WRR(I)=WCR(MT)

ENDIF
ENDIF
30 CONTINUE
RETURN
C

----- START FROM DRYING SCANNING CURVE -----

WRR(I)=WCR(MT)
IF(P(I).GE.0.0) THEN
  WSS(I)=WCSD(MT)
ELSE
  WSS(I)=(WC(I)-WCR(MT)*(1.-SEW))/SEW
  WSS(I)=MIN(WSS(I),WCSD(MT))
ENDIF
ENDIF

ELSEIF(KAPPA(I).EQ.1) THEN
  SEW=(1.+(AW(MT))*FR)**(BW(MT)-1.)
  IF(WC(I).LT.1.0E-10) THEN
    WSS(I)=WCSW(MT)
    WC(I)=WRR(I)+(WSS(I)-WRR(I))*SEW
  ELSE
    ----- START FROM WETTING BOUNDARY -----
    WSS(I)=WCSW(MT)
    IF(P(I).GE.0.0) THEN
      WRR(I)=WCR(MT)
    ELSE
      IF(WCSW(MT).LT.WCSD(MT)) THEN
        TERM=1./(WCSD(MT)-WCW(MT))-1./(WCSD(MT)-WCR(MT))
        WCW=WCSD(MT)-(WCSD(MT)-WC(I))/(1.+TERM*(WCSD(MT)-WC(I)))
      ELSE
        WCW=WCSD(MT)
      ENDIF
      WRR(I)=(WC(I)-WCW*SEW)/(1.-SEW)
    ENDIF
    WRR(I)=MAX(WRR(I),WCR(MT))
  ENDIF
ENDIF

C

----- CHECK WATER CONTENTS ----- 

IF(WC(I).LT.1.0E-10.OR.P(I).GT.0.0) GO TO 30

WCD=WCR(MT)+*(WCW(MT)-WCR(MT))*(1.+(AW(MT)*P(I))**BW(MT))
+ **(1./BW(MT)-1.) - SMALL

WCD=WCR(MT)+(WCSD(MT)-WCR(MT))*(1.+(AD(MT)*P(I))**BD(MT))
+ **(1./BD(MT)-1.) + SMALL

IF(WC(I).GT.WCD) THEN
  WRITE(KOUT,1022) Z(I),WC(I),WCD
  WC(I)=WCD
ELSEIF(WC(I).LT.WCW) THEN
  WRITE(KOUT,1024) Z(I),WC(I),WCW
  WC(I)=WCW
ENDIF

30 CONTINUE 
ENDIF
RETURN 

C

SUBROUTINE FLOW(KRAIN, KDRAIN, NIT, ISTEP, VALMN, VALNN, PET, RAIN, DRAIN, STOT, DELT, SUMT, WP)

PURPOSE: TO SOLVE THE FLOW EQUATION

---

IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION CP(200,2), CAP(201), COND(201)
EQUIVALENCE (CP(1,1), CAP(1)), (COND(1), A(1))
COMMON/STOR/ T(201), P(201), A(201), D(201), S(201), C1(201), C2(201)
COMMON/VAINON/MAT(201), KAPPA(201), P(201), PE(201), WC(201), WCE(201)
COMMON/GPTNO/IHKOD, IKHOD, ICOKOD, IKUKOD, IUPKOD, ILKOD, ICOKD, IBCKOD,
+ IOKOD, IRKOD
COMMON/GPVR/NE, NN, NSTEPS, NMAT, NLAYR, NBC, NPRINT, CNN, TDEPTH
COMMON/GPFOR/DELM, DELMN, DEMAX, TMX, TOL1, TOL2, NITMAX
+ WSC(5)
COMMON/UNITS/KTERM, KIN, KOUT, KPLT, KOB
DATA SMALL/1.0E-10/, EMAX/50.0/

--- SET WEIGHTING FACTOR FOR CONDUCTIVITY WEIGHTING ------
IF(IUPKOD.EQ.0) THEN
UPW=0.0
ELSE
UPW=1.0
ENDIF

--- DYNAMIC PART OF PROGRAM ------
NIT=NN-1
NIT=0
10 NIT=NIT+1
DO 12 I=1,NN
T(I)=PE(I)
S(I)=0.0
P(I)=0.5*(PE(I)+P(I))
12 CONTINUE

--- EVALUATE NODAL CONDUCTIVITY VALUES ----
PR=P(I)
IF(ITKOD.EQ.1) PR=PE(I)
COND(I)=HYPR(PR,2,I)
WCE(I)=HYPR(PR(I),1,1)
IF(ILLKOD.EQ.1) THEN

--- EVALUATE NODAL CAPACITIES FOR L2 LUMPING ----
IF(ITKOD.EQ.1) THEN
CAP(I)=0.0
ELSE
DWC=WCE(I)-WC(I)
DLP=PE(I)-P(I)
IF(ABS(DLP).GE.3.*TOL2) THEN
  CAP(I)=DWC/DLP
ELSE
  CAP(I)=HYPR(F(I),3,I)
ENDIF
ENDIF
CONTINUE
12 IF(ILKOD.EQ.0) THEN
C --- EVALUATE NODAL CAPACITY VALUES FOR LI LUMPING ----
DO 14 I=1,NE
IF(ITKOD.EQ.1) THEN
  CP(I,1)=0.0
  CP(I,2)=0.0
ELSE
  DELZ=DZ(I)
  I1=I+1
  DWC=WCE(I1)-WC(I)
  DWC1=WCE(I1)-WC(I1)
  DLP=PE(I1)-P(I1)
  DLP1=PE(I1)-P(I1)
  IF(ABS(2.*DLP+DLP1).GE.3.*TOL2) THEN
    CP(I,1)=3.*DWC/(2.*DLP+DLP1)*DELZ/DLT
  ELSE
    CP(I,1)=HYPR(F(I),3,1)*DELZ/DLT
  ENDIF
  IF(ABS(DLP+2.*DLP1).GE.3.*TOL2) THEN
    CP(I,2)=3.*DWC1/(DLP+2.*DLP1)*DELZ/DLT
  ELSE
    CP(I,2)=HYPR(F(I1),3,1)*DELZ/DLT
  ENDIF
ENDIF
14 CONTINUE
ENDIF
C ----- CALCULATE WATER UPTAKE-TERM ----
STOT=0.0
IF(IRUKOD.EQ.1.AND.PET.GT.0.0) THEN
  DO 18 I=1,NN
  F(I)=PET*ROOT(I,F(I),C(I))
18 CONTINUE
STOT=TOTAL(T,S,DZ,NN)
ENDIF
IF(IUPKOD.EQ.1) THEN
C ----- COMPUTE WEIGHTED CONDUCTIVITY TERMS ----- 
U1=UPW
HD1=F(I)+DZ(1)
HD2=F(2)
IF(HDL.LT.HD2) U1=-U1
C1(I)=(1.+U1)*COND(1) + (1.-U1)*COND(2))/DZ(I-1)
DO 20 I=2,NE
   HD1=F(I-1)+DZ(I-1)
   HD2=F(I)
   HD3=F(I+1)-DZ(I)
   U1=UPW
   IF(HD2.GT.HD1) U1=-U1
   U2=UPW
20 CONTINUE
U2=UPW
HDNE=F(NE)
HDNN=F(NN)-DZ(NN)
IF(HDNN.GT.HDNE) U2=-U2
C2(NE)=(1.+U2)*COND(NE) + (1.-U2)*COND(NN))/DZ(NE)
ELSE
   C1(I)=(COND(I-1)+COND(I))/DZ(I-1)
   C2(I)=(COND(I)+COND(I+1))/DZ(I)
22 CONTINUE
C2(NN)=(COND(NE)+COND(NN))/DZ(NE)
ENDIF

C

C --- COMPUTE CONDUCTIVITY WITHOUT UPSTREAM WEIGHTING ---
   C1(I)=(COND(I-1)+COND(I))/DZ(I)
   C2(I)=(COND(I)+COND(I+1))/DZ(I)
22 CONTINUE
C2(NN)=(COND(NE)+COND(NN))/DZ(NE)
ENDIF

C

C ---- CONSTRUCT GENERAL MATRIX EQUATION -----
IF(ILKOD.EQ.0) THEN
   F(I)=2.*CP(1,1)+CP(I-1,2))/6.
   A(I)=0.5*CI(I)
   D(I)=A(I)+F(I)
   DO 24 I=2,NE
      F(I)=(CP(I-1,1)+2.*CP(I-1,2)+2.*CP(I,1)+CP(I,2))/6.
      A(I)=0.5*C2(I)
      D(I)=0.5*(C1(I)+C2(I))+F(I)
24 CONTINUE
C2(NN)=(CP(NE,1)+2.*CP(NE,2))/6.
ELSE
   F(I)=0.5*CAP(I)*DZ(I)/DELT
   A(I)=0.5*CI(I)
   D(I)=A(I)+F(I)
   DO 28 I=2,NE
      F(I)=0.5*CAP(I)*(DZ(I-1)+DZ(I))/DELT
      A(I)=0.5*C2(I)
      D(I)=0.5*(C1(I)+C2(I))+F(I)
28 CONTINUE
C2(NN)=0.5*CAP(NN)*DZ(NE)/DELT
ENDIF

C

C1=A(NE)
FNN=F(NN)
D(NN)=A(NE)+F(NN)
C
--- INCLUDE SOIL SURFACE BOUNDARY CONDITION ---
IF(KRAIN.EQ.1) GO TO 38

34 PE(1)=VALN1
RAIN=D(1)*PE(1)-F(1)
F(1)=PE(1)
AT1=A(1)
A(1)=0.
D(1)=1.
F(2)=F(2)-AT1*PE(1)
GO TO 39

38 RAIN=VALN1
F(1)=F(1)+RAIN

C
--- INCLUDE LOWER BOUNDARY CONDITION ---
40 IF(KRAIN.EQ.1) 40,42,44
40 PE(NN)=VALNN
DRAIN=F(NN)-D(NN)*PE(NN)
F(NN)=PE(NN)
D(NN)=1.
F(NE)=F(NE)-ANE*PE(NN)
A(NE)=0.
GO TO 45

42 DRAIN=VALNN
F(NN)=F(NN)-DRAIN
GO TO 45

44 DRAIN=F(NN)
D(NN)=A(NE)
F(NN)=0.

C
--- SOLVE FOR THE NEW PRESSURE HEAD VALUES ---
45 DO 46 I=2,NN
R=A(I-1)/D(I-1)
D(I)=D(I)-R*A(I-1)

46 F(I)=F(I)-R*F(I-1)
PE(NN)=F(NN)/D(NN)
DO 48 I=2,NN
J=NN-I+1

48 PE(J)=(F(J)-A(J)*PE(J+1))/D(J)

C
--- CHECK ITERATIVE PROCESS ---
EPSN=0.0
NODEF=0
SP=1.0
ICONV=1
DO 52 I=1,NN
D(I)=PE(I)-T(I)
ABS=ABS(D(I))
TOT=TOT1*ABS(T(I))+TOL2
IF(ABS.D.R110) ICONV=0
IF(ABS.D.RABS(EPSN)) THEN
  EPSN=R(L)
  NODEP=I
ENDIF

52 CONTINUE
IF(I(ICONV.EQ.1)) THEN
  IF(KRAIN.NE.1) RAIN=RAIN+AT1*PE(2)
  IF(KDRAIN.EQ.0) DRAIN=DRAIN-ANE*PE(NN)
  IF(KDRAIN.EQ.2) DRAIN=DRAIN-PE(NN)*FNN
  IF(ITBK00.EQ.1) THEN
    WRITE(KOUT,1072) NIT
    NIT=1
  ENDIF
ENDIF
RETURN
ELSEIF(NIT.GE.NITMAX) THEN
  WRITE(KOUT,1034) SUMT,DELT,NODEP,PE(NODEP),T(NODEP),WP
  IF(ITBK10.EQ.1) THEN
    WRITE(KOUT,1070) NITMAX
    STOP 'MAXIMUM ITERATION NUMBER REACHED; EXECUTION ABORTED'
  ENDIF
  DELT=.5*DELT
  SUMT=SUMT-DELT
  IF(DELT.GT.DE2MIN) GO TO 58
  OLDT=SUMT-DELT

C 54 CONTINUE
C 55 --- WRITE RESULTS FOR LAST CONVERGED TIME VALUE ----
  IF(INKOD.EQ.0) THEN
    WRITE(KOUT,1050) OLDT
    DO 55 I=1,NN
      WRITE(KOUT,1055) Z(I),P(I),WC(I)
    ENDW
  ELSE
    WRITE(KOUT,1060) OLDT
    DO 56 I=1,NN
      WRITE(KOUT,1065) Z(I),P(I),WC(I),KAPPA(I)
    ENDW
  ENDIF
  CONTINUE

56 ENDIF
  STOP 'DELT IS LESS THAN DE2MIN, EXECUTION TERMINATED'
  DO 58 I=1,NN
      PE(I)=.5*(P(I)+PE(I))
    NIT=0
    GO TO 10
  ENDW
  ELSE

58 ENDIF

C 59 --- PREPARE FOR NEXT ITERATION ----
  IF(NIT.GT.1) SP=EPSN/(WP*EPS)
  SPABS=ABS(SP)
  WTEMP=1.0/(2.0*SPABS)
  IF(SP.GE.-1.0) WTEMP=(3.+SP)/(3.+SPABS)
  IF(WTEMP*ABS(EPSN).LE.EPMAX) THEN
    WP=WTEMP
  ELSE
    WP=EPMAX/ABS(EPSN)
  ENDIF
ENDIF
EPS=EPSN
DO 70 I=1,NN
PE(I)=+1*WP*D(I)
IF(ITKOD.EQ.1) P(I)=PE(I)
70 CONTINUE
GO TO 10
ENDF

-----
1034 FORMAT(/5(1H),': CONVERGENCE FAILURE AT TIME ',1PE10.4,', DELT=',
+1PE10.3,1X,5(3H),'/X,''NODE=',I3,' PE=',1PE10.3,', T=',1PE10.3,
+'' WP=',1PE10.3)
1050 FORMAT(/4X,'NODAL VALUES AT LAST TIME (SUM=','PE10.3,')/'
+1 ' Z PR. HEAD WC')
1055 FORMAT(2(1PE10.3,1X,0PF7.4)
+1 ' Z PR. HEAD WC KAPPA')
1060 FORMAT(/4X,'NODAL VALUES AT LAST TIME (SUM=',1PE10.3,')/'
+1 ' Z PR. HEAD WC KAPPA')
1065 FORMAT(2(1PE10.3,1X,0PF7.4,15)
+1 ' Z PR. HEAD WC KAPPA')
1070 FORMAT(/10X,'NO CONVERGENCE OF STEADY STATE FLOW SOLUTION AFTER'
+15,' ITERATIONS')
1072 FORMAT(/10X,'STEADY STATE FLOW SOLUTION PERFORMED IN',15,
+15 ' ITERATIONS')
END

C ----- SUBROUTINE UPDATE
C PURPOSE: TO CHECK FOR HYSTERETIC REVERSAL AND UPDATE
C MODEL PARAMETERS AND NODAL WATER CONTENTS
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VALNOD/MAT(201),KAPPA(201),P(201),PE(201),WC(201),WCE(231)
+1 C(201),CE(201),WSS(201),WRR(201),Z(201),DZ(200)
+1 COMMON/GPTWO/ITKOD,IHOKD,ICOKD,IRUKOD,IOPKOD,IKOKD,ICKOD,ICBOKD,
+1 IQOKD,IRKOKD
COMMON/GPHR/NE,NN,NSTEPS,NMAT,NLAYR,NBC,NPRINT,CNN,TDEPTH
COMMON/GPFOR/DELIN,DELMIN,DELMAX,TMAX,TOL1,TOL2,NITMAX
COMMON/GPFIN/AD(5),BD(5),WCSD(5),WCR(5),SATR(5),ANW(5),BNW(5),
+WCSW(5)

C
IF(ITKOD.EQ.0) GO TO 200
C
----- CHECK FOR REVERSAL ----- 
DO 100 I=1,NN
MT=MAT(I)
SMALL=-0.01/AD(MT)
DELP=P(I)-PE(I)
IF(DELP/FLOAT(KAPPA(I)) .LT.TOL2.OR.P(I).GE.SMALL) GO TO 100
C
----- WCN IS WATER CONTENT AT REVERSAL POINT -----
WCN=WC(I)
KAPPA(I)=-1*KAPPA(I)
C
----- UPDATE WCU = WATER CONTENT AT ZERO PRESSURE HEAD -----
IF(ABS(WCSW(MT)-WCSD(MT)) .LT.1.0E-10) THEN
WCU=WCSD(MT)
ELSEIF(P(I).LT.SMALL) THEN
TERM=1./(WCSD(MT)-WCSW(MT))-1./(WCSD(MT)-WCR(MT))
WCU=WCSD(MT)-(WCSD(MT)-WCN)/(1.+TERM*(WCSD(MT)-WCN))
WCU=MAX(WCU,WCSW(MT))
ELSE
WCU=WCN
ENDIF
C

----- UPDATE WSS AND WER -----  
IF(KAPPA(I).EQ.1) THEN
C

----- WETTING BRANCH -----  
WSS(I)=WCU
IF(P(I).LT.SMALL) THEN
SEW=1.+(AEM(T)*P(I)**BW(MT))**BW(MT)-1.
WRW(I)=(WCU-WCUF)*SEW/(1.-SEW)
WRW(I)=MAX(WRW(I),WCR(MT))
ELSE
WRW(I)=MIN(WRW(I),WCU)
ENDIF
ELSE
ENDIF
C

----- DRYING BRANCH -----  
WRW(I)=WCR(MT)
IF(P(I).LT.SMALL) THEN
SED=1.+(AD(T)*P(I)**BD(MT))**BD(MT)-1.
WSS(I)=WCR(MT)+(WCW-WCR(MT))/SED
WSS(I)=MIN(WSS(I),WCU)
ELSE
WSS(I)=WCU
ENDIF
ENDIF
C
100 CONTINUE
C

----- NODAL WATER CONTENTS AT NEW TIME LEVEL -----  
200 DO 210 I=1,NN
IF(P(I).LE.SMALL) THEN
MT=MAT(I)
IF(KAPPA(I).EQ.1) THEN
SE=1.+(AEM(T)*P(I)**BW(MT))**BW(MT)-1.
ELSE
SE=1.+(AD(T)*P(I)**BD(MT))**BD(MT)-1.
ENDIF
WCE(I)=WRW(I)+(WSS(I)-WRW(I))*SE
ELSE
WCE(I)=WSS(I)
ENDIF
C

----- RESET P AND WC FOR STEADY STATE FLOW -----  
IF(ITYRD.EQ.1) THEN
P(I)=PE(I)
WC(I)=WCE(I)
ENDIF
C
SUBROUTINE SOLUTE(RANO, DRANO, RAIN, DRAIN, CINO, CIN, QN1, QNN, DELT, VMAX, LINEAR)

* PURPOSE: TO ASSEMBLE AND SOLVE THE SOLUTE TRANSPORT EQUATION

IMPLICIT REAL*8 (A-H, O-Z)

LOGICAL LINEAR

DIMENSION CT(201), B(201), D(201), P(201), R(201), DC(201), Q(201)

COMMON/VALNOD/MAT(201), KAPPA(201), P(201), PE(201), WC(201), WCE(201)

, C(201), CE(201), WSS(201), WRR(201), Z(201), DZ(200)

COMMON/GPTWO/ITKOD, IHKOD, TCOKOD, IHUKOD, ITKOD, ILKOD, ICOKOD, IBCKOD,

+ IOKOD, IGBKOD

COMMON/GPTHRM/NN, NNSTEPS, NMAT, NLAYR, NBC, NPRINT, CNN, TNDFP

COMMON/GPSIX/AD(5), BD(5), WCSD(5), WCR(5), SATK(5), AN(5), BW(5),

+ WCSS(5)

COMMON/GPSIX/CTOL, DIF(5), DISP(5), RFCCOF(5), EXPF(5), DONE(5), USUNK(5)

COMMON/UNITS/KTERM, KIN, KOUT, KPLT, KOBS

----

CL=CN

TFAC=1.0/(6.*DELT)

WCF=1.0

TVAL=FLOAT(1-ICOKOD)

NIT=0

----- START ITERATION -----  

2 NIT=NIT+1

DO 4 I=1, NN

CT(I)=CE(I)

4 CONTINUE

----- CONSTRUCT RHS OF MATRIX EQUATION ----- 

IF (ITKOD.EQ.1) THEN

DRAIN=RAIN

DO 5 I=1, NN

Q(I)=RAIN

5 CONTINUE

ELSE

Q(I)=RANO

DO 6 I=2, NE

Q(I)=HYPR(P(I), 2, I)*(1.-(P(I+1)-P(I-1))/((DZ(I-1)+DZ(I))))

6 CONTINUE

Q(NN)=DRANO

ENDIF

DO 8 I=1, NN

MT=MAT(I)

CMID=0.5*(C(I)+CE(I))

IF (CMID.GT.0.0) THEN

PPAC=RFCCOF(MT)*CMID**(EXPF(MT)-1.)

ELSE

PPAC=0.0

ENDIF

8 CONTINUE
FFAC=RFQOF(MT)
ENDIF
RFAC=WC(I)+FEXP(MT)+FFAC
DECAY=DONE(MT)+WC(I)+DSONE(MT)+FFAC
DC(I)=DIF(MT)+WC(I)+DISP(MT)+ABS(Q(I))+Q(I)*2*DELT/(6.*RFAC)
R(I)=RFAC-0.5*DECAY*DELT
8 CONTINUE
D2=-0.25*(DC(I)+DC(2))/DZ(I) + (2.*Q(1)+Q(2))/12. +
+ TFAC*DIS(I)*R(I)+R(2))
AT2=0.25*(DC(I)+DC(2))/DZ(I) + (Q(I)+2.*Q(2))/12.
F(I)=D2*C(I) + AT2*C(2)
FNI=F(I)
IF(Q(I).GT.0.) F(I)=F(I)+0.125*Q(I)*(3.*CINO+CIN)*TVAL
DO 10 I=2,NE
B2=0.25*(DC(I-1)+DC(I))/DZ(I-1) + (2.*Q(I-1)+Q(I))/12.
D2=-0.25*(DC(I-1)+DC(I))/DZ(I-1) + (Q(I-1)+2.*Q(I))/12.
AT2=0.25*(DC(I-1)+DC(I))/DZ(I) + (Q(I)+2.*Q(I-1))/12.
F(I)=B2*C(I-1) + D2*C(I) + AT2*C(I-1)
10 CONTINUE
B2=0.25*(DC(NE)+DC(NN))/DZ(NE) + (2.*Q(NE)+Q(NN))/12.
D2=-0.25*(DC(NE)+DC(NN))/DZ(NE) + (Q(NE)+2.*Q(NN))/12.
+ TFAC*DS(NE)*R(NE)+2.*R(NN))
F(NN)=B2*C(NE)+D2*C(NN)
FNN=F(NN)
IF(DRAIN.LT.0.0) F(NN)=F(NN)-DRAIN*CL

------ CONSTRUCT RHS OF MATRIX EQUATION ------
IF(ILKGD,NE,1) THEN
Q(1)=RAIN
DO 12 I=2,NE
Q(I)=HYPR(PE(I),2,I)*(1.-PE(I)+PE(I-1))/
+ (DZ(I-1)+DZ(I)))
12 CONTINUE
Q(NN)=DRAIN*EF
IF(Q(I).GT.0.) F(I)=F(I)+0.125*Q(I)*(CINO+3.*CIN)*TVAL
VMAX=0.0
DO 14 I=1,NN
MT=MAX(I)
CMID=0.5*(C(I)+CE(I))
TF(NMT,GT,0.0) THEN
FFAC=RFQOF(MT)+CMID*(FEXP(MT)-1.)
ELSE
FFAC=RFQOF(MT)
ENDIF
RFAC=WC(E)+FEXP(MT)+FFAC
DECAY=DONE(MT)+WC(E)+DSONE(MT)+FFAC
DC(I)=DCE(I)+DIF(MT)+DISP(MT)+ABS(Q(I))-Q(I)*2*DELT/(6.*RFAC)
R(I)=RFAC + 0.5*DECAY*DELT
VMAX=ABS(MAX(Abs(Q(I))/RFAC)
14 CONTINUE
D(1)=0.25*(DC(I)+DC(2))/DZ(I) + (2.*Q(1)+Q(2))/12. +
+ TFAC*DIS(I)*(2.*R(I)+R(2))
DN1=D(1)
A(I)=0.25*(DC(I)+DC(2))/DZ(I) + (Q(I)+2.*Q(2))/12.
AN1=A(1)
DO 16 I=2,NE
B(I)=0.25*((DC(I-1)+DC(I))/DZ(I-1) - (2.*Q(I-1)+Q(I)))/12.
D(I)=0.25*((DC(I-1)+DC(I))/DZ(I-1)+((DC(I)+DC(I+1))/DZ(I)) +
+ (Q(I+1)-Q(I-1))/12. +
+ TFAC*(DZ(I-1)*(R(I-1)+2.*R(I))+DZ(I)*(2.*R(I)+R(I+1)))
A(I)=0.25*(DC(I)+DC(I+1))/DZ(I) + (Q(I)+2.*Q(I+1))/12.
16 CONTINUE
B(NN)=0.25*(DC(NE)+DC(NN))/DZ(NE) - (2.*Q(NE)+Q(NN))/12.
BNH=B(NN)
D(NN)=0.25*(DC(NE)+DC(NN))/DZ(NE) - (Q(NE)+2.*Q(NN))/12. +
+ TFAC*DZ(NN)*(R(NE)+2.*R(NN))
DNN=D(NN)
C
----- UPPER BOUNDARY CONDITION ----- 
IF(ICOKOD.EQ.1) THEN
  D(1)=1.0
  A(1)=0.0
  F(1)=0.0
  R(1)=0.0
ENDIF
C
----- INCLUDE LOWER BOUNDARY CONDITION FOR DOWNWARD FLOW ----- 
IF(Q(NN).GT.1.E-10) THEN
  B(NN)=1.0
  D(NN)=1.0
  F(NN)=0.0
ENDIF
C
----- SOLVE FOR NEW VALUES OF C ----- 
R(1)=F(1)
DO 18 I=2,NN
  G(I)=D(I-1)/D(I)
  D(I)=D(I)-G*A(I-1)
  R(I)=F(I)-G*R(I-1)
  IF(ABS(R(I)).LT.1.0E-30) R(I)=0.0
18 CONTINUE
C
C
CE(NN)=R(NN)/D(NN)
DO 20 I=2,NN
  J=NN-I+1
  CE(J)=(R(J)-A(J)*CE(J+1))/U(J)
20 CONTINUE
C
----- CHECK CONVERGENCE ----- 
IF(.NOT.LINEAR) THEN
  DO 24 I=1,NN
    IF(ABS(CE(I)-CT(I)).GT.CTOL) GO TO 30
24 CONTINUE
ENDIF
QMN=DN1*CE(1)+AN1*CE(2)-FN1
QNN=FNH-BNN*CE(NN)-DNN*CE(NN)
RETURN
NO CONVERGENCE

IF(NIT.GT.20) THEN
  STOP 'NO CONVERGENCE IN SOLUTE'
ELSE
  GO TO 2
ENDIF

DONE
END

SUBROUTINE TNEW(IS,NIT,INES,N,RK,RK,RK,D,D,SUM,VAL1,VAL1,+
  CIN,PET,DLMAX,VMAX)

PURPOSE: TO SET NEW DELT AND UPDATE BOUNDARY CONDITIONS
FOR NEXT TIMESTEP

IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VALMOD/MAT(201),KAPPA(201),P(201),PE(201),WC(201),WCE(201)+
  ,C(201),CE(201),WSS(201),WER(201),Z(201),DZ(200)+
  ,TIKOD,IKOD,IKOKOD,IKUKOD,IKKOD,IKKOD,IKKOD,
  WC(5)
COMMON/GPSEV/COTL,DIF(5),DISP(5),RFCOP(5),FEXP(5),DON(5),DSO(5)+
  ,CN1(51),POTET(51)
COMMON/GPEN/BCIN(51),IRTYP(51),IRTYP(51),BCN1(51),BCN(51),+
  CN1(51),POTET(51)

SET NEW VALUE FOR DELT
C INEW IS SET TO 1 IF NEW TIMESTEP WILL END AT BOUNDARY
C CONDITION CHANGE

IF(INEW.EQ.0) THEN
  DELCH=1.0
  DZAVE=ABS(Z(NN)-Z(1))/NE
  IF(VMAX.GT.0.0) DLMAXX=MIN(0.5D0*DZAVE/VMAX,DLMAXX)
  IF(NIT.LE.2) DELCH=1.25
  IF(NIT.GE.6) DELCH=0.80
  DELCH=MIN(DELCH,DLMAX/DELT)
  DELTN=DELT*DELCH
  IF((SUM+1.4*DELT) .GE. BCIN(IS+1)) THEN
    INEW=1
    DELTN=BCIN(IS+1)-SUM
    DELCH=DELTN/DELT
  ELSE
    DELCH=MIN(DELCH,DLMAX)
    INEW=0
    CUMIN=0.0
  ENDIF

UPDATE BOUNDARY CONDITIONS & RESET DELT

IS=IS+1
DLMAX=DELCH
INES=INES
CUMIN=0.0
PULS=1.0
IF(IRTPY(IS).EQ.2) THEN
   PULS=BCN1(IS)
   BCN1(IS)=0.0
   CUMIN=0.0
   DLMAXX=MIN(DLMAXX,0.1D0*PULS/SATK(MAT(1)))
ENDIF
DELCH=0.0
C
C ----- RESET DELT DEPENDING ON SURFACE BOUNDARY CONDITION CHANGE ----- 
IRESET=1
IF(IS.GE.2) THEN
   IF((ITKOD.EQ.1.OR.IBKOD.EQ.1) IRESET=0)
   IF(ITKOD(IS).EQ.IRTYP(IS)) THEN
      IF(ABS(BCN1(IS-1)).GT.1.0E-10) THEN
         RATIO=BCN1(IS)/BCN1(IS-1)
      ELSEIF(BCN1(IS).NE.BCN1(IS-1)) THEN
         RATIO=2.0
      ELSE
         RATIO=1.0
      ENDIF
      IF(RATIO.GT.0.0.AND.RATIO.LE.1.1) IRESET=0
   ENDIF
ENDIF
IF(IRESET.EQ.1) THEN
   DELTN=DELT
ELSE
   DELTN=MIN(DELT,BCTIM(IS+1)-SUMT)
ENDIF
C
C ----- UPDATE DEPENDENT VARIABLES ----- 
IF(ITKOD.EQ.1) DELCH=0.0
DO 85 I=1,NN
   DELP=(PE(I)-P(I))*DELCH
   DELC=(CE(I)-C(I))*DELCH
   P(I)=PE(I)
   WC(I)=WCE(I)
   C(I)=CE(I)
   PE(I)=P(I)+DELP
   CE(I)=C(I)+DELC
85 CONTINUE
C
C ----- UPDATE BOUNDARY CONDITIONS ----- 
KRAIN=IRTPY(IS)
KORAIN=IRTPY(IS)
IF(IBKOD.EQ.0) THEN
   VALN1=BCN1(IS)
   VALNN=BCNN(IS)
   CIN=CN1(IS)
   PET=POTET(IS)
ELSE
  TINT=(SUMT-BCTIM(IS))/(BCTIM(IS+1)-BCTIM(IS))
  VALN=TINT*BCNH(IS+1)+(1.-TINT)*BCNH(IS)
  VALN=INT*BCNH(IS+1)+(1.-INT)*BCNH(IS)
  PET=TINT*POTET(IS+1)+(1.-TINT)*POTET(IS)
ENDIF

C ---- DO NOT CHANGE BC FOR FLOW IF FLOW IS STEADY ----
IF(TKOD.EQ.1) THEN
  KRAIN=INTYP(1)
  KDRAIN=IDRYP(1)
  VALN=BCNH(1)
  VALN=BCNH(1)
  PET=POTET(1)
ENDIF
RETURN
END

-------------------------------------------------------------------------

C PURPOSE: TO CALCULATE THE ROOT EXTRACTION TERM
C
C IMPLICIT REAL*8 (A-H,0-Z)
C COMMON/GPENT/NRZ,APAR1,APAR2,APAR3,RDNOD(201)
C
C ------ RDF IS RELATIVE ROOT DENSITY ------
C
C ------ CALCULATE THE STRESS RESPONSE FUNCTION ----- PS=1.0+((PM+APAR1*C)/APAR2)**APAR3
C
C RETURN
END

C FUNCTION TOTAL(T,DZ,NN)
C
C PURPOSE: TO INTEGRATE T OVER SOIL DEPTH
C
C IMPLICIT REAL*8 (A-H,0-Z)
C DIMENSION T(201),DZ(200)
C
C TOTAL=0.0
C DO 5 I=1,NN-1
C    I=I+1
C   TOTAL=TOTAL+0.5*DZ(I)*(T(I)+T(I+1))
C 5 CONTINUE
C RETURN
END

C-------------------------------------------------------------------------

C PURPOSE: TO EVALUATE SOIL HYDRAULIC PROPERTIES
**ARGUMENTS:**

PR = PRESSURE HEAD AT HALF TIME LEVEL
N = INDEX FOR DESIRED FUNCTION,
   = 1: EVALUATE WATER CONTENT AT NODE I
   = 2: EVALUATE CONDUCTIVITY AT NODE I
   = 3: EVALUATE CAPACITY AT NODE I
I = NODAL INDEX

**IMPLICIT REAL*8 (A-H,O-Z)**

COMMON/VALNOD/MAT(201),KAPPA(201),P(201),PE(201),WC(201),WCE(201) + ,C(201),CE(201),WSS(201),WRR(201),Z(201),DZ(200)
COMMON/GPTWO/IKRDK,IKRDK,IKRDK,IKRDK,IKRDK,IKRDK,IKRDK,IKRDK, + IKRDK,IKRDK
COMMON/GPTHR/WN,NN,NSTEPS,NMAT,NLAYR,NBC,NPRINT,CNN,TDEP
DATA ZERO/0.0/,SMALL/1.0E-07/

MT=MAT(I)
IF(PR.GE.ZERO) GO TO 20
PT=PR
IF(KAPPA(I).EQ.1) THEN
  RA=AW(MT)
  RN=BN(MT)
ELSE
  RA=AD(MT)
  RN=BD(MT)
ENDIF
SE=(1.+(RA*PT)**RN)**(1./RN-1.)
WCT=WRR(I)+(WSS(I)-WRR(I))*SE
IF(N.EQ.1) THEN

**WATER CONTENT**

HYPR=WCT
ELSEIF(N.EQ.2) THEN

**CONDUCTIVITY**

EM=1.-1./RN
RWC=(WCT-WCR(MT))/(WCSD(MT)-WCR(MT))
RWC=MIN(RWC,1.0D0)
T=1.-(1.-RWC**(1./EM))**EM
IF(RWC.LT.0.04) T=EM*RWC**(1./EM)
HYPR=CATK(MT)*SQRT(RWC)*T*T
ELSEIF(N.EQ.3) THEN

**CAPACITY**

T=1.+(RA*PT)**RN
T1=(RA*PT)**(RN-1.)
CP=(WSS(I)-WRR(I))*T**((1./RN-2.)*(RN-1.))*RA*T1
HYPR=CP+WCT/WSS(I)*SMALL
ENDIF
RETURN
C ----- ZERO OR POSITIVE PRESSURE HEAD ----

20 IF(N.EQ.1) THEN
   HYPR=WSS(I)
ELSEIF(N.EQ.2) THEN
   HYPR=SATK(MT)
ELSEIF(N.EQ.3) THEN
   HYPR=SMALL
ENDIF

RETURN

END

*******************************************************************************

C PURPOSE: TO WRITE NODAL VALUES

*******************************************************************************

C
C IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VALMOD/MAT(201), KAPPA(201), P(201), PE(201), WC(201), WCE(201)
+ C(201), CE(201), WSS(201), WRR(201), Z(201), DZ(200)
COMMON/CPTWO/TKRD, THRD, ICOKD, IRKRD, IKRD, JPRHD, ILKRD, IDKRD, IBDKRD,
+ IOKRD, IRKRD
COMMON/GFTHR/NE, NN, NSTEPS,NMAT, NLAYR, NBC, NPRINT, CNN, TDEPTH
COMMON/UNITS/XTERM, KIN, KOUT, KPLT, KRB

*******************************************************************************

C IF(ITKRD.EQ.0) THEN
   IF(IHKRD.EQ.0) THEN
      WRITE(KOUT,1002)
      WRITE(KOUT,1004) (Z(I),P(I),WC(I),I=1,NN)
   ELSE
      WRITE(KOUT,1006)
      WRITE(KOUT,1008) (Z(I),KAPPA(I),P(I),WC(I),I=1,NN)
   ENDIF
   ELSE
   IF(IHKRD.EQ.0) THEN
      WRITE(KOUT,1010)
      WRITE(KOUT,1012) (Z(I),P(I),WC(I),C(I),I=1,NN)
   ELSE
      WRITE(KOUT,1014)
      WRITE(KOUT,1016) (Z(I),KAPPA(I),P(I),WC(I),C(I),I=1,NN)
   ENDIF
   ENDIF
   IF(IOKRD.EQ.1) THEN
      WRITE(KPLT,1018) TIME
      DO 10 I=1,NN
      WRITE(KPLT,1020) P(I),WC(I),C(I),Z(I)
   10 CONTINUE
   ENDIF

RETURN

*******************************************************************************

C ----- FORMATS -----

1002 FORMAT('1X,3( Depth P WC',3X)/)
1004 FORMAT('1X,0PF8.2,1PE10.3,0PF8.4,2X'))
1006 FORMAT('1X,3('' Depth Kappa P WC',3X)/)
C PURPOSE: TO WRITE OBSERVATION POINT VALUES

C IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION PRO(10),WCO(10),CO(10)
COMMON/VALNOD/MAT(201),KAPPA(201),P(201),PE(201),WC(201),WCE(201)
+       ,C(201),CE(201),WSS(201),WBR(201),Z(201),DZ(200)
COMMON/GPTWO/ITKOD,IKHOD,IKCOKD,IRKOD,UPKOD,ILAIK,IKCOD,IKBKOD,
+       IKOKD,IRSKOD
COMMON/UNITS/KTERM,KIN,KOUT,KPLT,KBRS
COMMON/GPMLP/NBRS,ZNBS(10),JBS(10),JBS(10,2),FBRS(10)

C ----- DO 20 I=1,NBRS
IMIN=I=1,NBRS
IPLS=I=1,NBRS
FAC=FBRS(1)
FAC=1.,-FAC
PRO(I)=FAC*PE(IMIN)+FAC1*PE(IPLS)
WCO(I)=FAC*WCE(IMIN)+FAC1*WCE(IPLS)
20 CONTINUE
IF(ITKOD.EQ.0) THEN
WRITE(KOBRS,1000) TIME,(PRO(I),I=1,NBRS)
WRITE(KOBRS,1002) (WCO(I),I=1,NBRS)
ELSEIF(ITKOD.EQ.1) THEN WRITE(KOBRS,1004) TIME,(CO(I),I=1,NBRS)
ELSEIF(ITKOD.EQ.2) THEN WRITE(KOBRS,1000) TIME,(PRO(I),I=1,NBRS)
WRITE(KOBRS,1002) (WCO(I),I=1,NBRS)
WRITE(KOBRS,1006) (CO(I),I=1,NBRS)
ENDIF
C ------- RETURN

C ----- FORMAT(5X,F10.4,10F11.2)
C ------- FORMAT(5X,F10.4,10F11.3)
C ------- FORMAT(5X,F10.4,10F11.4)
C ------- FORMAT(15X,10F11.4)