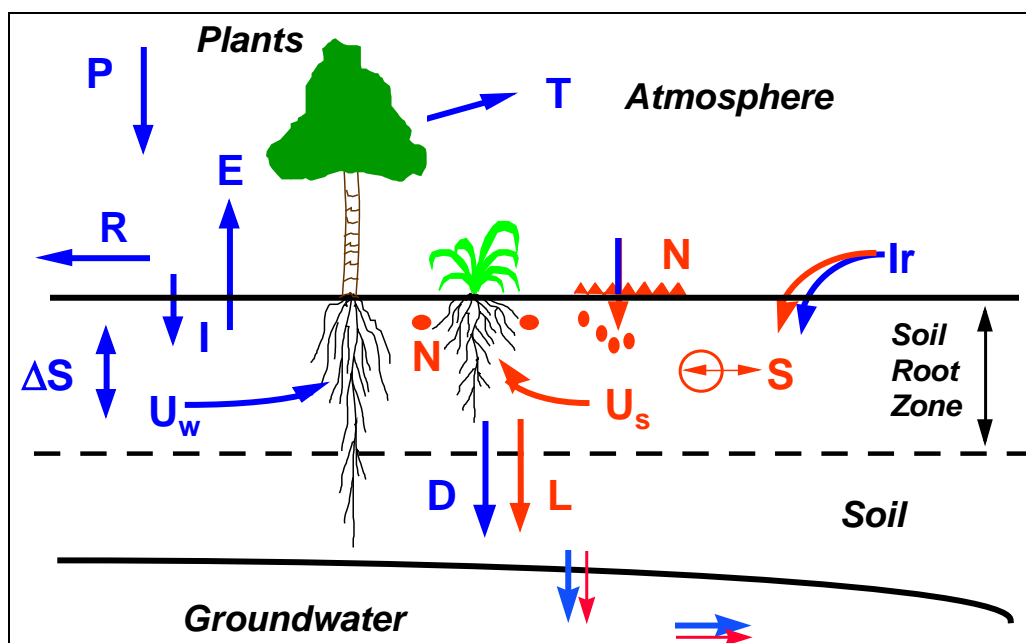


DIVISION OF SOILS

Divisional Report

SWIMv2.1 User Manual

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Caring for Australia's Soils

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INTRODUCTION

SWIM is an acronym that stands for Soil Water Infiltration and Movement. It is a software package developed within the CSIRO Division of Soils for simulating infiltration, evapotranspiration, and redistribution. The first version (SWIMv1) was published in 1990 (Ross, 1990b). Version 2 of the model (identified as SWIMv2.0), which combines water movement with transient solute transport and which accommodates a variety of soil property descriptions and more flexible boundary conditions, was completed in 1992. The latest version, SWIMv2.1, is described in this manual.

SWIMv2 is based on a numerical solution of the Richards' equation and the advection-dispersion equation. It can be used to simulate runoff, infiltration, redistribution, solute transport and redistribution of solutes, plant uptake and transpiration, soil evaporation, deep drainage and leaching. The physical system and the associated flows addressed by the model are shown schematically in Fig.1. Soil water and solute transport properties, initial conditions, and time dependent boundary conditions (e.g., precipitation, evaporative demand, solute input) need to be supplied by the user in order to run the model.

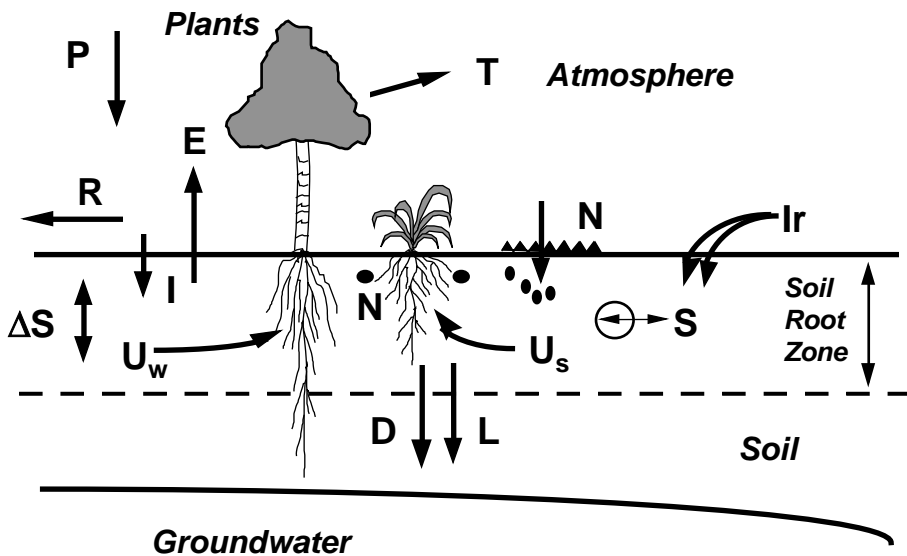


Figure 1: Components of the soil water and solute balances addressed by SWIMv2.1;
 P = precipitation, R = runoff, I = infiltration, U_w = water uptake, U_s = solute uptake, T = transpiration, E = evaporation, D = drainage, L = solute leaching, Ir = irrigation/fertilization, N = nutrients/fertiliser, ΔS = storage, S = solute source/sink.

The model deals with a one-dimensional soil profile. For a vertical soil profile, this means that it may be vertically inhomogeneous, but must be horizontally uniform. This assumption has two consequences of importance in many common simulations. There is only one hydraulic conductivity function for each soil layer, so that any macropore, or bypass, flow can only be accounted for in a limited way. Secondly, the calculated solute concentrations apply to the whole soil layer, which means that there is no concentration gradient from the bulk soil to near the root surface. The presence of such a concentration gradient may in reality affect the soil osmotic potential and hence water and solute uptake.

The major features common to the SWIMv1 and SWIMv2 models include the ability to deal with (Bristow *et al.* 1994; Smettem *et al.*, 1994)

- layered and gradational soils such as occur in field soils where hydraulic properties vary with depth down the profile, either abruptly or gradually,
- saturated/unsaturated conditions as can occur at layer interfaces, which result in locally perched water,
- surface ponding as can occur under high rainfall intensities,
- surface runoff, where ‘excess’ water can be removed from the system,
- surface sealing, where the properties of the surface may vary directly as a function of rainfall energy, and hence as a function of time,
- rainfall dynamics, so that real storm intensities (down to 1-minute resolution and below) can be simulated.

The main differences between SWIMv1 and SWIMv2.1 are

- SWIMv2.1 includes solute transport,
- SWIMv2.1 has a more flexible description of hydraulic properties and boundary conditions than SWIMv1,
- vapour flow, hysteresis, bypass flow, osmotic effects, and potential subsurface downslope flow are included in SWIMv2.1,
- specifications of root length density with depth and time, and potential plant water uptake with time are more complete and flexible in SWIMv2.1 than in SWIMv1,
- several parameters that used to be “hard-wired” in SWIMv1 are now accessible in the SWIMv2.1 input file,
- SWIMv2.1 allows for ‘cultivations’ or ‘disturbances’ of the soil surface which enable the application of dry fertiliser (solute) and resetting of the surface conductance and surface roughness values at specified times.

The overall purpose of the model is to address issues relating to the soil water and solute balance. As such it is a research tool that can be integrated in laboratory and field studies concerned with soil water and solute transport. We believe, however, that the model is also eminently suitable for management and education. The recent implementation of SWIMv2 into the Agricultural Production Systems sIMulator (APSIM-SWIM) (Huth *et al.*, 1996; McCown *et al.*, 1996) will further enhance its use in these areas.

SWIMv1 has already been used world-wide in a variety of studies (e.g. Cresswell *et al.*, 1992; Bond *et al.*, 1994; Barkle *et al.*, 1995; Bristow *et al.*, 1995; Koolen *et al.*, 1996). Version 2.1 is currently being tested and validated “in-house”, but has already been successfully applied in a field study of bromide leaching (Bond *et al.*, 1997) and, as APSIM-SWIM, in a study of bromide and nitrate leaching under sugarcane (Verburg *et al.*, 1996).

This manual consists of three parts. The first part covers the theoretical background of the many features of SWIMv2.1. Precise instructions for preparation of the input files and running the model are given in Part II. The two parts are linked by the reference in Part II to equations used in Part I, and by the use of input parameter names of Part II (printed in **bold** face) in Part I. Part II also contains some examples, that illustrate different aspects of the model input and output. Part III consists of four appendices, including a list of publications related to SWIMv1, SWIMv2 and APSIM-SWIM.

Both SWIMv2.1 and this manual need to be viewed as “dynamic” documents that will be updated as our understanding of the soil water and solute balances improves. We would, therefore, appreciate any comments or feedback that users may have. As with SWIMv1, SWIMv2 was originally written assuming that a preprocessor would be used to interface with the user. A preprocessor is not yet available; hence current data input facilities are less than ideal.

Acknowledgments

The development of SWIMv2.1 has benefited greatly from the input of users of SWIMv1 and SWIMv2.0. In particular the authors wish to acknowledge the feed-back from Warren Bond, Hamish Cresswell, Neil Huth, Brian Keating, Zahra Paydar, Keith Smettem and Val Snow. They also made valuable comments on this User Manual.

The SWIMv2 program was written by Peter Ross, who also wrote the HYPROPS program described in Section II.2. This latter program is used to generate the required soil hydraulic property input data. Steve Bailey and Peter Ross wrote the SWIMPLOT program described in Section II.3. It uses the binary output file of SWIMv2.1 to generate graphical output. Warren Bond wrote the SWIMREAD program (Section II.4) to extract data from the binary output file and provide it in a format ready for use in spreadsheets. Their help with these user-interfaces is greatly appreciated.

Thanks also to Jody Biggs who prepared the final graphs for publication in this user manual.

SWIMv2.1 User Manual

I - THEORETICAL BACKGROUND

1. WATER MOVEMENT

1.1 Richards' equation

One-dimensional flow of water through isothermal, rigid, unsaturated or saturated soil is governed by Darcy's law (Darcy, 1856; Buckingham, 1907)

$$q = -K \frac{dH}{dx} \quad (1)$$

where

- q = water flux density = volumetric water flow per unit cross-sectional area per unit time
[cm³ water/cm² soil/h]
 K = hydraulic conductivity [cm² water/cm soil/h]
 H = hydraulic head [cm water]
 x = distance into the soil [cm soil]

Darcy's law states that water flows down a hydraulic gradient at a rate proportional to the gradient. The "constant" of proportionality, K , varies with conditions such as soil type and water content, but not with the gradient. Darcy's law has proven to be valid under most conditions of soil water flow provided the soil can be treated as a continuum, i.e., provided a suitable length scale for definition of variables such as q , K , and H can be established (Bear, 1979).

In flow situations where q , K , and H vary in time and space, so-called transient water flow, it is necessary to combine Darcy's equation with the continuity equation that conserves mass of water. For a fluid of constant density, this is expressed as conservation of volume

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial x} + S \quad (2)$$

where

- θ = volumetric water content [cm³/cm³]
 t = time [h]
 S = source (or sink, if negative) strength [cm³ water/cm³ soil/h]

Combining Eq. (1) and (2) gives the Richards' equation (Richards, 1931)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(K \frac{\partial H}{\partial x} \right) + S \quad (3)$$

In rigid, unsaturated or saturated soil in which the gas pressure is always atmospheric (i.e. air can move freely) the hydraulic head, H , is the sum of the gravitational potential, z , and the matric potential, ψ (which for convenience is extended to include positive values under saturated conditions). The gravitational potential, z , is equal to the elevation from some arbitrary reference level. The Richards' equation then becomes:

* The units in this manual reflect as much as possible those of the SWIMv2.1 code, namely cm for distance and h for time.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} K \left(\frac{\partial \psi}{\partial x} + \frac{dz}{dx} \right) + S \quad (4)$$

where θ and ψ are related by the water retention curve (Section I.2.1) and K is related to θ by the hydraulic conductivity function (Section I.2.2). This so-called mixed θ and ψ form of the Richards' equation can be conveniently solved numerically using the Newton-Raphson iterative method (see e.g. Campbell, 1985). The numerical solution accurately conserves water during numerical solution, no matter how large the time step (Hornung and Messing, 1981; Milly, 1984; Celia *et al.*, 1990; Ross, 1990a; Ross and Bristow, 1990).

Equation (4) is highly non-linear, especially in dry soils, where K and ψ change over several orders of magnitude with changes in θ . SWIMv2.1, therefore, solves the Richards' equation by using a hyperbolic sine transform of ψ (Ross, 1990a). For this purpose Eq. (4) is written as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} K \left(\frac{d\psi}{dp} \frac{\partial p}{\partial x} + \frac{dz}{dx} \right) + S \quad (5)$$

with

$$\begin{cases} -\frac{\psi - \psi_0}{\psi_1} = \sinh p & \psi < \psi_0 \\ -\frac{\psi - \psi_0}{\psi_1} = p & \psi \geq \psi_0 \end{cases} \quad (6)$$

where ψ_0 (**psi0**) and ψ_1 (**psi1**) are shifting and scaling parameters, respectively. Appropriate choice of ψ_0 allows the inverse hyperbolic sine transform to be applied over the dry range $\psi < \psi_0$ while using a linear transform for the wet range $\psi \geq \psi_0$. Ross (1990a) obtained good results with $\psi_0 = -50$ cm and $\psi_1 = -5$ cm. Both $d\psi/dp$ and $d^2\psi/dp^2$ are continuous functions of p over the entire range of ψ (Ross, 1990a), which is desirable for the Newton-Raphson method. Use of this transform allows SWIMv2.1 to deal with unsaturated and saturated flow and dry soils with relatively large space steps in the numerical solution.

Equation (5) does not specify the direction of flow relative to the direction of gravity. Directions of flow other than vertical flow are, therefore, possible. In the input file to SWIMv2.1 (see Section II.1.2) $(-dz/dx)$ is set equal to the gravity factor **gf**, which is equal to the cosine of the angle between the x -direction and gravity. A gravity factor of 1 gives vertical downward flow, a gravity factor of 0 gives horizontal flow (gravity ignored). Note, however, that flow is still strictly one-dimensional and that lateral flow is not taken into account.

Regarding water flow SWIMv2.1 includes a number of simplifications and approximations:

- Only one-dimensional flow is considered. Lateral equilibrium is, therefore, assumed. Net lateral surface runoff is treated as a sink terms at the surface.
- Macropores and bypass flow are only taken account of in a limited way (see Section I.2.5).
- The soil matrix is assumed rigid, so that SWIMv2.1 is not strictly applicable to swelling soils.
- Soil air flow is ignored.
- Vapour flow within the soil can be included as part of the conductivity term, but only in response to matric potential gradients (see Section I.2.4).

- Temperature effects on water movement are ignored.
- Osmotic effects are ignored, except in water uptake and soil evaporation (see Section I.4.4)
- Wetting front instability or fingering (Glass *et al.*, 1989; Hendrickx *et al.*, 1993) is not taken into account.

1.2 Numerical solution

For the purpose of numerically solving Eq. (5) with the Newton-Raphson method, the soil profile is represented by a series of nodes (Fig. 2); the number and spacing of which are determined by the user in the input file (see Section II.1.2). Smaller depth increments lead to more accurate solutions, but also cost more time (e.g. Ross, 1990a; Ross and Bristow, 1990). The first node defined by the user is always taken as the soil surface or top boundary. Equation (5) can then be discretised on a space-time grid given by the points (x_i, t_j) , $i = 0, 1, 2, \dots, n$, $j = 0, 1, 2, \dots, m$. The result is (Ross, 1990a)

$$\frac{\theta_i - \theta_i^j}{\Delta t} = \frac{1}{\Delta x_i} \left[(Kd)_{i+1/2} \frac{p_{i+1} - p_i}{\Delta x_{i+1/2}} - K_{i+1/2} g - (Kd)_{i-1/2} \frac{p_i - p_{i-1}}{\Delta x_{i-1/2}} + K_{i-1/2} g \right] + S_i \quad (7)$$

where

$$d = d\psi/dp \quad (8)$$

$$g = -dz/dx \text{ (gf)} \quad (9)$$

$$\Delta t = t_{j+1} - t_j \quad (10)$$

$$\Delta x_i = (x_{i+1} - x_{i-1})/2 \quad (11)$$

$$\Delta x_{i+1/2} = x_{i+1} - x_i \quad (12)$$

$$Kd_{i+1/2} = 0.5K_i d_i + 0.5K_{i+1} d_{i+1} \quad (13)$$

$$K_{i+1/2} = \sigma K_i + (1 - \sigma) K_{i+1} \quad (14)$$

and σ a space-weighting factor (see below). Similar definitions apply for $\Delta x_{i-1/2}$, $(Kd)_{i-1/2}$, and $K_{i-1/2}$. A backward difference or fully implicit form in time has been used. All quantities given are for time t_{j+1} except θ_i^j , which is the water content at (x_i, t_j) .

The time step Δt is set so that the greatest water flux in the system will not be more than a specified value (the “water increment parameter” **dw**), unless the minimum time step size (**dtmin**) has been reached. Small steps are, therefore, used when conditions are changing rapidly during intense rainfall or when the soil is saturated, while large steps (up to a maximum time step size **dtmax**) are used when conditions are changing slowly such as when the soil is dry.

The space-weighting factor σ for gravity flow in Eq. (14) can in principle vary between 0 and 1. In SWIMv2.1 the user can vary σ (**swt**) between 0.5 (central space weighting) and 1.0 (fully upstream weighting), or choose the option of central space weighting until possible oscillation begins (**swt=0**) (see also Chapter I.6). Central space weighting tends to give smaller numerical errors than fully upstream weighting (Ross, 1990a).

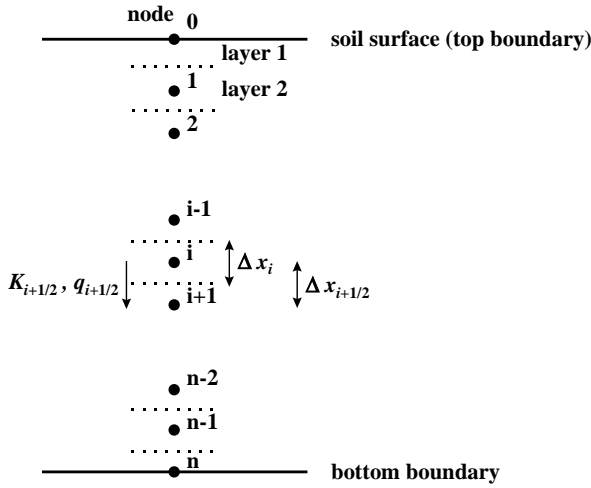


Figure 2: Discretisation of space in SWIMv2.1

1.3 Initial and boundary conditions and source/sink terms

Solution of Eq. (5) requires the specification of initial conditions, boundary conditions and the source/sink term S . The initial condition can be given as matric potential or water content at specified depths. If initial water contents are specified (see Section II.1.2), then these are converted by SWIMv2.1 to matric potentials using the specified water retention curve. Boundary conditions for Eq. (5) can in general be defined in terms of matric potentials, potential gradients or fluxes, all defined as functions of time.

Top boundary

One of the options in SWIMv2.1 is to define a constant potential top boundary conditions (**itbc=1**), where the matric potential at the surface node is kept constant at the value given in the initial profile. Water needed to keep this value constant is “created” if necessary. The boundary acts as a source of water and the water is artificially “extracted” from or added to an imaginary runoff. This may lead to negative values being reported for runoff.

Flux type boundary conditions are set by appropriate choices of rainfall/irrigation and potential evaporation intensities. These conditions may, however, be modified if the soil hydraulics are limiting (even in the case of an infinite surface conductance (**itbc=0**)), or if there is a surface seal of limited conductance (conductance function, **itbc=2**). In both cases not all water may infiltrate immediately. SWIMv2.1 gives three options to handle this deficit in infiltration

- no ponding, all water runs off (**isbc=0**)
- ponding, no runoff (**isbc=1**)
- simple power-law runoff function (**isbc=2**)

If a fourth option (**isbc=3**) is chosen, surface runoff is treated as for **isbc=2**, but SWIMv2.1 will also calculate potential subsurface downslope flow (see below).

The conductance (**itbc=2**) and runoff (**isbc=2** and **isbc=3**) functions are explained in more detail in Sections I.5.2 and I.5.3, respectively.

Bottom boundary

SWIMv2.1 gives four options for the bottom boundary condition:

- given matric potential gradient of variable magnitude in time (**ibbc=0**)
- given potential, variable in time (**ibbc=1**)
- zero flux (**ibbc=2**)
- seepage, with threshold suction variable in time (**ibbc=3**)

If **ibbc=0**, then $d\psi/dx$ needs to be specified as a function of time (**ntb**, **tb(1,i)**, **tb(2,i)**). When unit gradient of hydraulic head is chosen, $d\psi/dx = 0$ (**tb(2,i)=0**). If **ibbc=1**, then ψ needs to be specified as a function of time (**ntb**, **tb(1,i)**, **tb(2,i)**). This option is useful for simulating measured values or a (fluctuating) water table (e.g. time record of positive values for ψ). Note, however, that this condition can cause the bottom boundary to act as a source of water (similar to the top boundary condition **itbc=1**). If **ibbc=2**, then $q = 0$ (Eq. 1). This can be used to simulate an impermeable layer. If **ibbc=3**, then upward flow through the bottom boundary is not possible and drainage will only occur when ψ exceeds the specified limit (**ntb**, **tb(1,i)**, **tb(2,i)**). Contrary to the situation with **ibbc=1**, the drained water is in this case lost to the system. Laboratory columns in which the base is held at a certain suction (e.g. by use of a suction plate, wick, or simply open to the air) are represented by this boundary condition.

Source/sink terms

The source/sink term S in Eq. (5) can be root water uptake, soil evaporation (surface node only), or bypassing of water to a certain node. These source/sink terms are discussed in Sections I.4.3, I.4.2, and I.2.5, respectively.

Potential subsurface downslope flow

For information only, SWIMv2.1 calculates the potential downslope flux density at node i , q_{Li} , using Darcy's Law applied to the gravitational component of the hydraulic head only:

$$q_{Li} = -K_i \frac{dz_i}{dw} = K_i \frac{s}{\sqrt{1+s^2}} \quad (15)$$

where

- q_{Li} = potential downslope flux density at node i [$\text{cm}^3/\text{cm}^2/\text{h}$]
 K_i = hydraulic conductivity at node i [cm/h]
 z_i = gravitational potential at node i [cm]
 w = distance in downslope direction [cm]
 s = slope gradient [cm/cm]

Because q_{Li} is in the downslope direction (w), Eq. (15) is obtained by considering only the component of the gradient in gravitational potential in the direction of w . Figure 3 illustrates that $-dz_i/dw$ is equal to the cosine of the angle between the w -direction and gravity (i.e. $\cos(\alpha)$), which is in turn equal to the sine of the slope angle β and hence related to the slope gradient s .

The potential subsurface downslope flux is integrated over the profile depth to give the total potential subsurface downslope flow [cm^3/cm width of slope/h]. Integration of time gives the cumulative value that is reported in the output of SWIMv2.1 [cm^2]. Note that only potential flow is given. It is currently not a sink in the water balance!

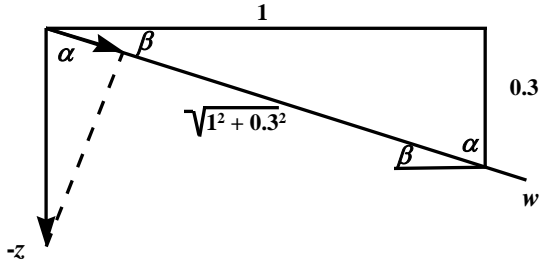


Figure 3: Example of subsurface downslope flow geometry for $s=0.3$. See text for explanation of symbols.

1.4 Changes from SWIMv1

- Vapour flow within the soil, which was not part of SWIMv1, is now included, but only in response to matric potential gradients (see Section I.2.4).
- Bypass flow has been added, but only in a limited way (see Section I.2.5)
- In SWIMv2.1 nodes can be placed on soil layer interfaces, allowing soil properties to change abruptly (see Chapter I.6).
- SWIMv2.1 includes a more flexible description of hydraulic properties than SWIMv1 (see Sections I.2.1 and I.2.2)
- SWIMv2.1 includes flexible boundary conditions as discussed in Section I.1.3. SWIMv1 used a more restrictive set with a conductance function (**itbc=2**) and a runoff function (**isbc=2**) as top boundary conditions. The bottom boundary condition in SWIMv1 was specified as drainage under gravity (**ibbc=0**, constant at zero matric potential gradient), drainage at a given potential (**ibbc=1**, constant at initial value), or zero flux (**ibbc=2**).

2. HYDRAULIC PROPERTIES

In unsaturated systems θ and ψ are related by the water retention curve (Section I.2.1), and K is related to θ by the hydraulic conductivity function (Section I.2.2). Both these functions are strongly non-linear. For saturated conditions these functions reduce to constants:

$$\begin{cases} \theta = \theta_s \\ K = K_s \end{cases} \quad (16)$$

where

- θ = volumetric water content [cm^3/cm^3]
- θ_s = saturated volumetric water content [cm^3/cm^3] (**ths**)
- K = hydraulic conductivity [cm/h]
- K_s = saturated hydraulic conductivity [cm/h] (**hks**)

2.1 Water retention curve

Instead of relating θ and ψ directly, SWIMv2.1 uses a normalised parameter S , the effective saturation.

$$S = (\theta - \theta_r) / (\theta_s - \theta_r) \quad (17)$$

where

- S = effective saturation [cm^3/cm^3]
- θ_r = residual volumetric water content [cm^3/cm^3] (**thr**)

The effective saturation, S , of a porous medium can be expressed as the cumulative distribution function of a capillary pore-size distribution (given as a function of the matric potential). Sometimes several partly overlapping pore-size distributions can be distinguished. This is, for example, the case for soils that exhibit the so-called matrix-macropore dichotomy (Clothier, 1990; Othmer *et al.*, 1991; Smettem and Ross, 1992). Following Ross and Smettem (1993), therefore, the water retention curve in SWIMv2.1 is described by considering it as the sum of overlapping pore-size distributions. The result is an overall water retention curve which can be expressed as a sum of simple functions. The parameters for these simple functions are input to the program HYPROPS (see Section II.2), which processes them to an overall water retention curve. The output generated by HYPROPS is used to prepare the input file for SWIMv2.1. HYPROPS offers a choice of models for these simple functions (**terms**). They are:

- unsmoothed Brooks-Corey (and Campbell) function (**fun=uc**)
- smoothed Brooks-Corey (and Campbell) function (**fun=bc**)
- modified, unsmoothed Brooks-Corey (and Campbell) function (**fun=um**)
- modified, smoothed Brooks-Corey (and Campbell) function (**fun=mc**)
- van Genuchten function (**fun=vg**)
- one-parameter exponential function (**fun=ex**)

The unsmoothed Brooks-Corey function (**uc**) is that of Brooks and Corey (1964, 1966):

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = S(\psi) = \begin{cases} \left(\frac{\psi}{\psi_e} \right)^{-1/b}, & \psi \leq \psi_e \\ 1, & 0 \leq \psi > \psi_e \end{cases} \quad (18)$$

where,

ψ = matric potential [cm] ($\psi \leq 0$)

ψ_e = air entry potential [cm] ($\psi_e \leq 0$)

b = constant

If $\theta_r = 0$, then this equation reduces to that of Campbell (1974, 1985). Equation (18) results in an unrealistic, sharp discontinuity at ψ_e . The smoothed Brooks-Corey function (**bc**) overcomes this by replacing the exponential function by a parabolic one near saturation. The equations were taken from Hutson and Cass (1987).

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = S(\psi) = \begin{cases} \left(\frac{\psi}{\psi_e} \right)^{-1/b}, & \psi \leq \psi_i \\ 1 - c\psi^2, & 0 \leq \psi > \psi_i \end{cases} \quad (19)$$

where,

$$a = 2b / (1 + 2b), \psi_i = \psi_e a^{-b} (\psi_i \leq 0), c = (1-a) / \psi_i^2$$

Neither Eq. (18) nor Eq. (19) predicts zero water content at oven dryness. Ross *et al.* (1991) overcame this problem by introducing a matric potential $\psi_0 = -10^7$ cm into the equations. The modified equations are given by

unsmoothed Brooks-Corey function (**um**)

$$S(\psi) = \begin{cases} \frac{|\psi|^{-1/b} - |\psi_0|^{-1/b}}{|\psi_e|^{-1/b} - |\psi_0|^{-1/b}}, & \psi \leq \psi_e \\ 1, & 0 \leq \psi > \psi_e \end{cases} \quad (20)$$

smoothed Brooks-Corey function (**mc**)

$$S(\psi) = \begin{cases} \frac{|\psi|^{-1/b} - |\psi_0|^{-1/b}}{|\psi_e|^{-1/b} - |\psi_0|^{-1/b}}, & \psi \leq \psi_i \\ 1 - c\psi^2, & 0 \leq \psi > \psi_i \end{cases} \quad (21)$$

where,

$$\psi_i = \psi_e ((2b/(2b+1))^{-b}), c = (1+a) / ((1+2b) \psi_i^2), a = 1 / ((\psi_e/\psi_0)^{-1/b} - 1)$$

The van Genuchten function (**vg**), from van Genuchten (1980), is written as:

$$S(\psi) = \left[1 + (\alpha |\psi|)^n \right]^{-m} \quad (22)$$

where α , m and n are constants; $\alpha > 0$ and $n > 1$.

The one-parameter exponential function (**ex**) was introduced for describing macroporosity (Ross and Smettem, 1993). It should only be used as an enhancement to a water retention curve, specifically for the region near saturation, and not as a water retention curve by itself.

$$S(\psi) = (1 + \alpha_{ex} |\psi|) \exp(-\alpha_{ex} |\psi|) \quad (23)$$

where α_{ex} is a constant.

The functions are summed according to:

$$S(\psi) = \sum_{i=1}^N \phi_i S_i(\psi) \quad (24)$$

where $S_i(\psi)$ is given by Eq. (18) - (23), ϕ_i the fraction (**tfac**) of each function in the overall water retention curve, and N is the number of terms (**nterms**). Of course, it is not required to sum multiple functions. By setting N equal to one, a straight forward Brooks-Corey or van Genuchten water retention curve can be defined.

2.2 Hydraulic conductivity function

The hydraulic conductivity function can be related to the overall water retention curve through the model of Mualem (1976) (**fun=mu**), or it can be defined following the models of Brooks and Corey (1964, 1966) (**fun=bc**) or van Genuchten (van Genuchten 1980; van Genuchten and Nielsen, 1985) (**fun=vg**). Equations (25) - (30) are from Ross and Smettem (1993).

The Mualem model (**mu**) relates the relative conductivity $K_r(\psi) = K(\psi)/K_s$ to the effective saturation S , via the equation

$$K_r(\psi) = S^p \left[g(\psi) / g(0) \right]^2 \quad (25)$$

where p is the pore interaction index (Mualem, 1976), and

$$g(\psi) = \int_{-x}^{\psi} \psi'^{-1} f(\psi') d\psi' \quad (26)$$

in which $f(\psi) = dS/d\psi$ and $S = S(\psi)$ is defined by Eq. (24). Note that $K \leq K_s$, so that $0 \leq K_r \leq 1$.

The Brooks-Corey hydraulic conductivity function (**bc**) is defined as

$$K_r(\psi) = S^{p+2+2b} \quad (27)$$

where p is the pore interaction index and $S = S(\psi)$ is given by Eq. (24). This equation is obtained by applying the Mualem model (1976) to the unsmoothed Brooks-Corey water retention curve

(Eq. 18) (see also Example 2.2 in Section II.2.3). When $p=1$, Eq. (27) is equivalent to those given by Brooks and Corey (1964, 1966) and Campbell (1974, 1985).

The van Genuchten model (**vg**) (van Genuchten, 1980; van Genuchten and Nielsen, 1985) is expressed as

$$K_r(\psi) = S^p \left[I_x \left(m+1/n, 1-1/n \right) \right]^2, n > 0 \quad (28)$$

in the general form, and

$$K_r(\psi) = S^p \left[1 - \left(1 - S^{1/m} \right)^m \right]^2, m = 1 - 1/n; n > 0 \quad (29)$$

as a more restricted case. $I_x(\cdot)$ is an incomplete beta function, p is the pore interaction index, and $S = S(\psi)$ is given by Eq. (24). Equations (28) and (29) correspond to applying the Mualem (1976) model to the Van Genuchten water retention curve given by Eq. (22).

Applying the Mualem (1976) model to the one-parameter exponential water retention function (**ex**) (Eq. 23) results in

$$K_r(\psi) = \left(1 - \alpha_{ex} \psi \right)^p \exp \left[(p+2) \alpha_{ex} \psi \right] \quad (30)$$

As well as the Mualem (1976) conductivity model, HYPROPS is set up such that the total porosity from θ_r to θ_s can consist of a number of non-interacting pore-spaces (**components**), whose conductivities are effectively in parallel (Ross and Smettem, 1993). In this case

$$K(\psi) = \sum_{i=1}^M K_{si} K_{ri}(\psi) \quad (31)$$

where

$K_i(\psi)$ = hydraulic conductivity function for pore-space i [cm/h]

K_{si} = saturated hydraulic conductivity of pore-space i [cm/h] (**hks**)

$K_{ri}(\psi) = K_i(\psi) / K_{si}$ = relative hydraulic conductivity function for pore-space i [-]

M = number of components (**nc**)

The summation of the hydraulic conductivities of the pore-spaces (Eq. 31) does not take the fraction of these pore-spaces (**cfrac**) explicitly into account. It is assumed that the effect of **cfrac** is included in the K_{si} (**hks**) given for each pore space (**component**) (see also Example 2.3 in Section II.2.3). When there are two or more independent pore-spaces defined, the overall water retention curve does take the fractions of the various components (**cfrac**) into account, in addition to the fractions of the various terms (**tfrac**):

$$S(\psi) = \sum_{j=1}^M \left[\varepsilon_j \sum_{i=1}^N \phi_i S_i(\psi) \right] \quad (32)$$

where

- ε_j = the fractional contribution of each component (**cfrac**)
 N = the number of terms (**nterms**)
 ϕ_i = the fraction (**tfac**) of each function in the overall water retention curve
 $S_i(\psi)$ = from Eq. (18)-(23)

The effect of multiple components on the overall conductivity function is shown in Fig. 4, where macropores cause the hydraulic conductivity to increase at low suction near saturation. When macropores are sparsely distributed in the soil, they may not significantly contribute to the water retention curve, but will still have a large effect on the hydraulic conductivity near-saturation (Clothier and Smettem, 1990; Smettem and Ross, 1992; Smettem and Kirkby, 1990). This can be achieved by setting **cfrac** of the macropore component equal to zero.

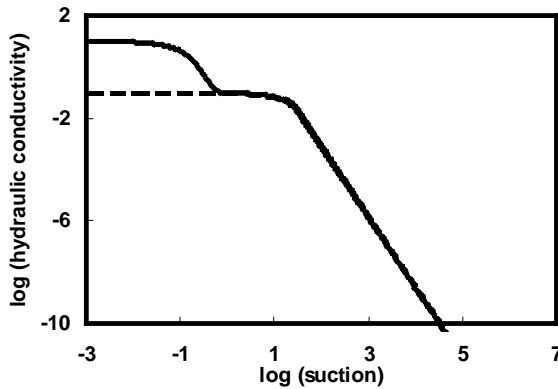


Figure 4: Matrix-macropore dichotomy effect on the hydraulic conductivity function. The dashed and continuous lines represent the matrix and the whole soil, respectively.

SWIMv2.1 requires as input (to HYPROPS) the parameters of the water retention and hydraulic conductivity functions as specified in Eq. (18)-(32). In other words, the values of the parameters (K_s , θ_s , θ_r , b and ψ_e , or α and n , ...) need to be determined before SWIMv2.1 and HYPROPS can be used. These values can be obtained by fitting experimental data (e.g., Milly, 1987; Leij *et al.*, 1992) or by estimation on the basis of so-called pedotransfer functions that use other data such as particle size distribution and bulk density (e.g., Rawls and Brakensiek, 1989; Vereecken *et al.*, 1989, 1990; Rawls *et al.*, 1991; Williams *et al.*, 1992; Tietje and Tapkenhinrichs, 1993; Smettem and Gregory, 1996). Combinations of the two are also possible (e.g., Chang and Uehara, 1992; Cresswell and Paydar, 1996; Paydar and Cresswell, 1996) and inverse modelling techniques can be used as well (e.g., Ross, 1993). Often unsaturated hydraulic conductivity data are not available, so that a relation with the water retention curve is assumed (e.g., $p=1$ in Eq. (25), (27) -(30); Campbell, 1974; Mualem, 1976; van Genuchten, 1980; Talsma, 1985). The accuracy with which the parameters need to be determined will depend on the type of soil, climate and scenario, as well as on the type and accuracy of the output required (e.g. Wösten *et al.*, 1990; Finke *et al.*, 1996; Verburg *et al.*, 1996a).

The overall water retention and hydraulic conductivity functions defined by the user are used in HYPROPS to generate a hydraulic property table based on a piecewise cubic approximation (Ross, 1992). This table, which is used as input for SWIMv2.1, contains $\log_{10}|\psi|$, water content θ , the slope of θ vs. $\log_{10}|\psi|$, $\log_{10} K$, and the slope of $\log_{10} K$ vs. $\log_{10}|\psi|$.

2.3 Conversion of hydraulic property description in SWIMv1

The equivalent of the hydraulic property description used in SWIMv1 is the smoothed Brooks-Corey water retention curve (**bc**) with the Brooks-Corey hydraulic conductivity function (**bc**). In SWIMv1 the hydraulic conductivity function was defined as

$$K = K_s \left(\frac{\theta}{\theta_s} \right)^{bn} \quad (33)$$

If $n=0$ was used, then this corresponds to using the **bc** function with pore interaction parameter $p=1$. If $n \neq 0$ was used, then in the SWIMv2.1 input file the pore interaction parameter p needs to be set equal to $b(n-2)-2$.

The extra term in the hydraulic conductivity function in SWIMv1 that was used to describe increased conductivity due to macropores

$$K = K_s \left(\frac{\theta}{\theta_s} \right)^{bn} + K_m \left(\frac{\theta}{\theta_s} \right)^{bm} \quad (34)$$

is in SWIMv2.1 represented by an extra **component**. This component has no water retention curve linked to it (by setting fractional contribution (**cfraction**) equal to zero (but keeping **nt**=1). The pore interaction parameter p needs to be equal to $b(m-2)-2$ (see Example 2.5 in Section II.2.3).

2.4 Vapour conductivity

In contrast to SWIMv1, SWIMv2.1 can account for isothermal vapour flow (**ivap**≠0 in input file, see Section II.1.2). This is vapour flow in response to gradients in the soil matric potential. Temperature and osmotic effects are ignored. A vapour conductivity is calculated according to Campbell (1985, Chapter 9) and added to the liquid conductivity in the transport equation (Eq. 5).

Derivation of vapour conductivity (from Campbell, 1985)

The flux density of vapour is described by Fick's law

$$f_v = -D_v \frac{1}{\rho_w} \frac{dc_v}{dz} \quad (35)$$

with

$$c_v = h c_v' \quad (36)$$

where

f_v	= flux density of vapour [cm/h]
D_v	= vapour diffusivity in the soil [cm ² /h]
ρ_w	= density of water ($1.0 \cdot 10^{-3}$) [kg/cm ³]
c_v	= soil vapour concentration [kg/cm ³]
c_v'	= saturation vapour concentration [kg/cm ³]
h	= relative humidity [-]

For the derivative with respect to depth in Eq. (35) we can apply the chain rule

$$\frac{dh}{dz} = \frac{dh}{d\psi} \frac{d\psi}{dz} \quad (37)$$

Further, because the relative humidity, h , is a function of the soil matric potential if $T=\text{constant}$

$$h = \exp(M_w \psi g / RT) \quad (38)$$

M_w	= mass of one mole of water (0.01802) [kg/mol]
ψ	= soil matric potential [cm]
g	= gravitational constant ($9.81 \cdot 10^2$) [cm/s ²]
R	= gas constant ($8.3143 \cdot 10^4$) [kg cm ² /s ² /mol/K]
T	= absolute temperature [K]

where we can write

$$\frac{dh}{d\psi} = h M_w g / RT \quad (39)$$

So that by combining Eq. (35) - (39) we obtain

$$f_v = -k_v \frac{d\psi}{dz} \quad (40)$$

where

$$k_v = D_v c_v' h g M_w / RT \quad (41)$$

is the vapour conductivity [cm/h] which can be added to the liquid conductivity to calculate the total water flux (liquid+vapour). In its calculations SWIMv2.1 assumes a temperature of 293K and a saturation vapour concentration of $0.017 \cdot 10^{-6}$ kg/cm³. The vapour diffusivity in the soil is obtained by multiplying the vapour diffusivity in free air (864 cm²/h) with a tortuosity coefficient (0.66) and the air-filled porosity (in SWIMv2.1 taken as $(\theta_s / 0.93 - \theta)$).

2.5 Macropores and bypass flow

Some effects of macropores can be accounted for in SWIMv2.1 through appropriate description of the water retention and hydraulic conductivity functions. For example, some macropores of small volume have a large effect on the hydraulic conductivity near saturation. This can be handled by adding a component to the description of the hydraulic conductivity function and using the simple one-parameter water retention function for this component (see Example 2.4 in Section II.2.3). Note that this inclusion of macroporosity is limited to the definition of the hydraulic conductivity and does not extend to the actual transport process. Actual bypassing of

water (and solutes) is not accounted for by this approach. In SWIMv2.1 it is assumed that the soil is a continuum for which the one-dimensional Richards' equation (Eq. 4) applies, so that only one hydraulic conductivity function is used per soil layer. This approach is useful as long as the macropores are in lateral equilibrium with water in the matrix, at the macro-scale. It is, therefore, limited to types of macroporosity that allow a hydraulic conductivity to be defined for the whole soil. If macropores are large and sparse, then the basic assumption of soil as a one-dimensional continuum is not met and Darcy's law and the one-dimensional Richards' equation are not strictly applicable.

To allow for actual bypassing of water and solutes, a separate function is included in SWIMv2.1 on an experimental basis (Fig. 5). When bypass flow is allowed to occur (**ibp**=1 in input file) water and dissolved solutes from runoff bypass the soil matrix to the node closest to the specified bypassing depth (**xbp**). SWIMv2.1 then sets the parameter **ibp** equal to the number of this node. This bypassing occurs only from runoff; therefore, if there is no runoff (either because the matrix absorbs all water, or because the surface condition is set to "ponding with no runoff" (**isbc**=1) (see Section I.1.3) then downward bypass flow will not occur. Bypass flow can also not occur with a constant potential top boundary condition (**itbc**=1, see Section I.1.3).

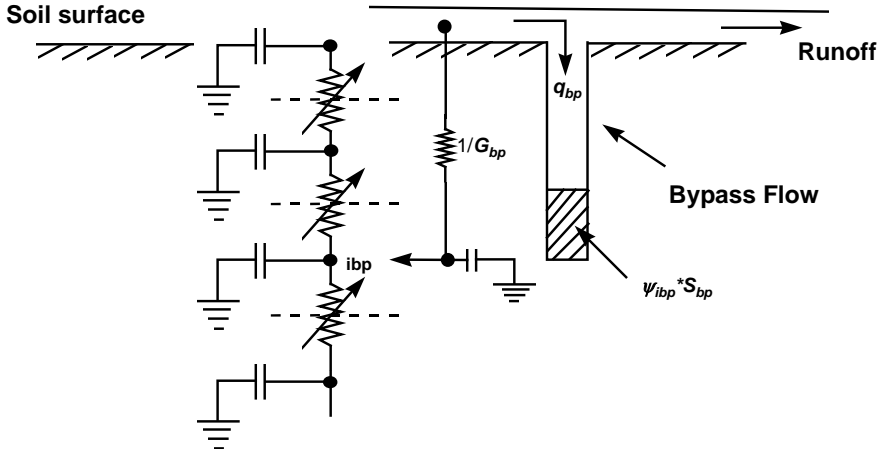


Figure 5: Schematic representation of bypass flow in SWIMv2.1

If there is no positive head at the bypass node **ibp** ($\psi \leq 0$), then bypass flow is like free flow down a tube:

$$q_{bp} = G_{bp} g (x_{ibp} - x_0) \quad (42)$$

where

- q_{bp} = bypass flux [cm/h]
- G_{bp} = conductance [1/h] (**gbp**)
- g = gravity factor (1 for vertical flow) [-] (**gf**)
- x_{ibp} = depth of bypass node **ibp** [cm]
- x_0 = depth of surface node [cm]

As shown in Eq. (42) $g(x_{ibp} - x_0)$ is the driving potential for bypass flow.

If there is a positive head at the bypass node **ibp** ($\psi_{ibp} > 0$), then this is assumed to be equivalent to water standing in the tube (cm water). A correction is made to Eq. (42) for this depth

$$q_{bp} = G_{bp} g \left(x_{ibp} - x_0 - \psi_{ibp} \right) \quad (43)$$

Equations (42) and (43) determine the potential bypass flow. If the rate of runoff $< q_{bp}$, then q_{bp} is set equal to the rate of runoff (i.e. there is no water left for runoff). If the rate of runoff $> q_{bp}$, then the rate of runoff is decreased by q_{bp} . It also follows from Eq. (42) and (43) that the gravity factor (**gf**) must be positive for bypass flow to occur (i.e. in horizontal flow systems bypass flow cannot occur). Note also that, as currently programmed, SWIMv2.1 allows upward flow to occur if $\psi_{ibp} > (x_{ibp} - x_0)$. This water is then added to the runoff. This has not been verified physically. It seems an unlikely situation.

At the bypass node **ibp**, the amount of bypass flow water is added as a source in the balance equations (as a sink in case of upward flow) (S in Eq. (4)). Instantaneous lateral distribution within the layer is assumed. If $\psi_{ibp} > 0$, then there is an additional water storage of $\psi_{ibp} S_{bp}$ at this node. The water can be visualised as stored in the bypass channel. Depending on the surface area of this bypass channel, this corresponds to more or less water (in cm) per cm of matric potential ψ . This is expressed in the input parameter S_{bp} (**sbp**), which has effectively the unit [cm of water in channel per cm of positive ψ per unit area]. Flow to and from this storage is accounted for in the balance equation of node **ibp** by treating it as an additional source or sink term. The additional water stored is documented separately in the output of SWIMv2.1.

2.6 Hysteresis

SWIMv2.1 allows soil-water hysteresis effects to be taken into account. The description of the hysteresis scanning curves is kept rather simple, because of the wide range of possible shapes for the water retention curve. It is assumed that the main drying curve (see Fig. 6a) is the one given by the hydraulic property data set in the input file. This curve is described according to one of the functions in Section I.2.1. The main wetting curve is then obtained by a shift **dh** either on a linear scale (Eq. (44), Fig. 6a) or on a log scale (Eq. (45), Fig. 6b).

$$\theta = h(\psi + \mathbf{dh}) \quad (44)$$

$$\log(\theta) = \log(h(\psi + \mathbf{dh})) \quad (45)$$

where h is the function chosen for the main drying curve. A shift on the log scale results in a hysteresis gap that becomes wider at large (negative) matric potentials (Fig. 6c). When the position of the main wetting curve is determined by a shift **dh** on a linear scale, then $\mathbf{dh} < 0$. If the shift **dh** occurs on a log scale, then $\mathbf{dh} > 1$. This corresponds to **dh** being a multiplier on the linear scale. If $0 < \mathbf{dh} < 1$, SWIMv2.1 assumes that the wetting curve is identical to the drying curve (no hysteresis). Primary scanning curves (those branching off the main wetting and drying curves) are described by cubic interpolation between points on the main wetting and drying curves, whereby the slopes at the intersections match those of the main wetting and drying curves (see Fig. 6d). Secondary and higher order scanning curves are not distinguished from the primary scanning curves, nor are the drying curves different from the wetting curves. In other words, $\psi(\theta)$ can “move” in both directions on the primary scanning curves.

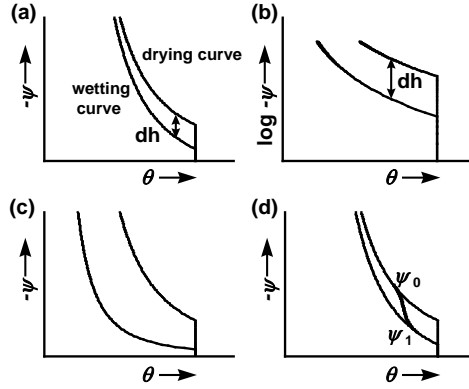


Figure 6: Definition of hysteresis in SWIMv2; (a) shift dh on linear scale, (b) shift dh on log scale and (c) corresponding plot on linear scale, and (d) scanning curves.

The shape of the scanning curves is determined by the parameter **hyscon**. Suppose a reversal from drying to wetting occurs at point ψ_0 on the main drying curve in Fig. 6d. Then, in the case of a linearly shifted wetting curve, the point where the scanning curve meets the main wetting curve, ψ_1 , is defined as

$$\psi_1 = \psi_0 - dh * \mathbf{hyscon} \quad (46)$$

For monotonicity of the cubic interpolation it is required that $\mathbf{hyscon} \geq 1.5$. The description of the cubic interpolation between ψ_0 and ψ_1 , which matches the slopes of the main hysteresis curves at these points, is based on a parameter z , which expresses the fractional distance of ψ between the main drying and wetting curves. It is defined as

$$z = (\psi - \psi_0) / (\psi_1 - \psi_0) \quad (47)$$

The cubic polynomial is expressed in terms of z and given by

$$f(z) = -dh * z * (\mathbf{hyscon} + z * (2*z-3)) \quad (48)$$

The scanning curves are then defined as

$$\theta = h(\psi_0 + f(z)) \quad (49)$$

where h is the function chosen for the main drying curve (from Section I.2.1). A similar derivation applies to scanning curves where the shift dh is on a log scale. In the input file for SWIMv2.1 **hyscon** also serves as flag for hysteresis: if **hyscon**=0, then no hysteresis is assumed.

The variable z in Eq. (47) is also used in SWIMv2.1 to keep track of where one is on the scanning curves. If $z = 0$, then we are on the main drying curve, if $z = 1$, then we are on the main wetting curve. A simulation run does not need to start on the main wetting or drying curves. The initial fractional distance of ψ between the main drying and wetting curve, z_{init} , can be specified in the input file (**fh**). See also Example 1.6 in Section II.1.3.

Confidence that this scheme will perform satisfactorily is based on the results of Jaynes (1985), who found that a similar, linear method gave equally good predictions as more complex hysteresis models. As with this linear method the scheme included in SWIMv2.1 does not result in a pumping effect when the pressure potential is varied cyclically (Hanks *et al.*, 1969).

3. SOLUTE TRANSPORT

3.1 Advection-dispersion equation

Solute transport is governed by two processes: diffusion and advection* with water. Differences in pore water velocities (both within an individual pore and between pores of different sizes) lead to an additional effect known as hydrodynamic dispersion. This process results in spreading of the solute, very much like diffusion does, so the two are often combined in the mathematical description of solute transport. In SWIMv2.1 solute movement is based on the following solute transport equation

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(\rho s)}{\partial t} = \frac{\partial}{\partial x} \left(\theta D \frac{\partial c}{\partial x} \right) - \frac{\partial(qc)}{\partial x} + \phi \quad (50)$$

where

- c = solute concentration in solution [μmol or μg solutes / cm^3 water]
- s = adsorbed concentration [$\mu\text{mol/g}$ soil or $\mu\text{g/g}$ soil]
- ρ = soil bulk density [g/cm^3] (**rhob**)
- t = time [h]
- x = depth [cm]
- θ = water content [cm^3/cm^3]
- q = water flux density [cm/h]
- D = combined dispersion and diffusion coefficient [cm^2/h]
- ϕ = source/sink term [$\mu\text{mol}/\text{cm}^3/\text{h}$ or $\mu\text{g}/\text{cm}^3/\text{h}$]
- and

$$D = \tau D_0 + \varepsilon |v|^n \quad (51)$$

$$\tau = a(\theta - b)^\xi \quad (52)$$

$$s = k c^\eta \quad (53)$$

where

- D_0 = ionic or molecular diffusion coefficient in free water [cm^2/h] (**d0**)
- τ = tortuosity factor [-]
- ε = dispersivity of the medium [$(\text{cm}^2/\text{h}) / (\text{cm}/\text{h})^n$] (**dis(i)**)
- v = pore water velocity = q/θ [cm/h]
- a = empirical constant [-] (**a**)
- b = empirical constant [-] (**dthc**)
- ξ = empirical constant [-] (**dthp**)
- n = empirical constant [-] (**disp**)
- k = coefficient of Freundlich isotherm [(mol or g adsorbed solute/g soil)/(mol or g solute/ cm^3 water) $^\eta$] (**exco**)
- η = power of Freundlich isotherm [-] (**fip(i)**)

* In the literature the advection process is also commonly referred to as convection, and the advection-dispersion equation as the convection-dispersion equation.

Currently, SWIMv2.1 can only account for one solute at a time. The choice of units for solute concentration, c , is flexible. Any units can be used as long as they are expressed in an amount/cm³ soil. Units of s , ϕ , and k change accordingly, as well as the units of **slos** (see Section I.4.4).

Values for the diffusion coefficient in water (**d0**) (Eq. 51) can be found in several literature sources (e.g., Robinson and Stokes, 1965; Lehrman, 1979; Weast and Astle, 1980; Kemper, 1986; Sadeghi *et al.*, 1988). The diffusion coefficient depends on the temperature, the concentration of the solute, and on the ions that the solute consists of. For example, if chloride moves as CaCl₂, it has a diffusion coefficient of approximately 0.045 cm²/h, whereas if it moves as KCl the appropriate value is about 0.071 cm²/h (25°C, approx. 1.0 μmol/cm³ (=0.001 M)). If there is a mixed electrolyte, the diffusion coefficient is determined by a contribution from each. Nye (1966) has outlined an approach to calculate the appropriate diffusion coefficient in that case (see e.g., Bond and Phillips, 1990a). If the cation and anion fronts move separately (e.g., Bond and Smiles, 1988; Bond and Phillips, 1990b), then the appropriate diffusion coefficient for the anion may be that in combination with the resident cation, rather than with the incoming cation. Note, however, that SWIMv2.1 currently does not handle separate fronts.

The equation for tortuosity (Eq. (52)) is general and allows flexible parameterisation. It is, for example, able to handle the commonly used relationship of Millington and Quirk (1961).

$$\tau = \theta^{7/3} / \theta_s^2 \quad (54)$$

For saturated systems τ is often taken to be a constant equal to 0.67 (Rose, 1977), although Bond (1986) obtained a value of 0.442 in a saturated breakthrough experiment. While there is evidence that suggests that τ is a function of water content in unsaturated soils (e.g., Porter *et al.*, 1960; Barraclough and Tinker, 1981), it has been assumed constant and equal to 1.0 in a number of successful descriptions of solute transport in unsteady, unsaturated flow experiments (Smiles *et al.*, 1981; Bond *et al.*, 1982; Bond *et al.*, 1997). In practice the difference in spreading resulting from values of τ between 1 and 0.5 is often small. Another frequently used equation for tortuosity was first proposed by Kemper and van Schaik (1966). Adapted to fit the definition of D and τ used by SWIMv2.1 it has the following functional form

$$\tau = \frac{a}{\theta} \exp(b\theta) \quad (55)$$

While this equation cannot be converted to Eq. (52), it can give an idea of the magnitude of τ . Comparing this equation with data collected on soils by Olsen *et al.* (1965) and Porter *et al.* (1960), Olsen and Kemper (1968) found that b was approximately 10 and $0.005 < a/\theta < 0.01$. They also point out, however, that this equation was applicable only in the range of moisture contents between 330 and 15000 cm suction. Indeed, at high water contents, values of τ above 1 may be obtained, and this is not consistent with the definition of τ .

Values for the dispersivity, ε , vary widely in the literature (see e.g., extensive review by Beven *et al.*, 1993). Values obtained in field experiments are commonly an order of magnitude higher than those obtained in laboratory field columns (approx. 1 cm) (Rose *et al.*, 1982). This is often a result of the inclusion of other effects in the dispersion term, such as heterogeneities in pore water velocities, preferential flow, and “immobile” water effects, because of using a steady-state analysis to fit the dispersion term to the field data. Spatial averaging of data and neglect of the

contribution of diffusion can play a role as well. When the average flow velocity is low, the choice of the dispersivity is less critical because the second term on the right hand side of Eq. (51) becomes small. The value of the exponent, n , is usually take to be 1, although higher values have been found and 1.2 is sometimes used.

Equation (53) is the Freundlich isotherm for adsorption. If $\eta = 1$, then this reduces to a linear isotherm. While Eq. (51), (52), and (53) have some physical basis, they are essentially empirical equations, so that the units in Eq. 51 and 53 vary with the powers n and η .

3.2 Numerical solution

For the discretisation of Eq. (50) in time, SWIMv2.1 uses backward differencing in time and central differences in space, as for the Richards' equation; however, for the convective term the Crank-Nicolson scheme is used and some upstream weighting can be added via a space weighting factor. The discretised form of Eq. (50) is

$$\frac{\theta_i c_i - \theta_i^j c_i^j}{\Delta t} + \rho \frac{s_i - s_i^j}{\Delta t} = \frac{1}{\Delta x_i} \left[(\theta D)_{i+1/2} \frac{c_{i+1} - c_i}{\Delta x_{i+1/2}} - (\theta D)_{i-1/2} \frac{c_i - c_{i-1}}{\Delta x_{i-1/2}} \right] - \frac{1}{\Delta x_i} \left[\frac{(qc)_{i+1/2} + (qc)_{i+1/2}^j}{2} - \frac{(qc)_{i-1/2} + (qc)_{i-1/2}^j}{2} \right] + \phi_i \quad (56)$$

where

$$\Delta t = t_{j+1} - t_j \quad (57)$$

$$\Delta x_i = (x_{i+1} - x_{i-1}) / 2 \quad (58)$$

$$\Delta x_{i+1/2} = x_{i+1} - x_i \quad (59)$$

$$(qc)_{i+1/2} = q_{i+1/2} [\sigma_s c_i + (1 - \sigma_s) c_{i+1}] \quad (60)$$

$$(\theta D)_{i+1/2} = \bar{\theta} \left(D_0 a (\bar{\theta} - b)^\xi + \bar{\varepsilon} \left(|q_{i+1/2}| / \bar{\theta} \right)^n \right) \quad (61)$$

$$\bar{\theta} = (\theta_i + \theta_{i+1}) / 2 \quad (62)$$

$$\bar{\varepsilon} = (\varepsilon_i + \varepsilon_{i+1}) / 2 \quad (63)$$

and σ_s a space-weighting factor (see below). Similar definitions apply for $\Delta x_{i-1/2}$, $(qc)_{i-1/2}$, and $(\theta D)_{i-1/2}$. All quantities given are for time t_{j+1} except when a superscript j is used to indicate that these quantities are given at time t_j .

The space-weighting factor σ_s (Eq. 60) can in principle vary between 0 and 1. In SWIMv2.1 the user can vary σ_s (**slswt**) between 0.5 (central space weighting) and 1.0 (full upstream weighting), or choose the option of central space weighting until oscillation begins (**slswt=0**), at which time the model adjusts towards upstream weighting. Central space weighting gives smaller numerical errors than full upstream weighting (see Chapter I.6 for details).

SWIMv2.1 solves the Richards' equation (including evaporation and plant water uptake) before solving the advection-dispersion equation. In Eq. (60) $q_{i+1/2}$, the flow between nodes x_i and x_{i+1}

(see Fig. 2), is therefore known. Note that where osmotic effects influence the solution of the Richards' equation, as in plant uptake and surface evaporation (see Section I.4.4), the solution concentrations at the beginning of the current time step are used.

Equation 53 is linear in the concentrations when there is no adsorption of the solute ($k = 0$) or when the adsorption isotherm is linear ($\eta = 1$). If the Freundlich isotherm is used ($\eta \neq 1$) then a Newton-Raphson iteration technique is used to solve the equations. During this process only the non-linear terms involving η need to be updated.

3.3 Solute initial and boundary conditions

Solute can be added to the system in a variety of ways:

- as part of initialisation: solute concentrations (in solution) are specified for each node (**csl(i)**). If there is adsorption ($k \neq 0$), then the initial amount of adsorbed solute is “created” using the specified adsorption isotherm.
- in rainfall or irrigation: cumulative solute additions (in amounts rather than concentrations) are given in the input file (**nts** time-addition pairs). These solute additions are assumed to be mixed with the rainfall/irrigation. The units of the amounts need to be consistent with the unit of solute concentration used. E.g. if, over a certain time period, 0.32 cm of irrigation water is applied to the soil surface (0.32 cm³ water/cm² surface area) with a solute concentration of 50 μmol solute /cm³ water, then the amount of solute added (to be specified in input file) is 16 μmol solute / cm² surface area (see also Example 1.7 in Section II.1.3).
- as part of cultivation (see Section I.5.4): in this case the solute is added “dry” to the surface. It will enter the soil with infiltrating water at a concentration of **slsci** or disappear with surface runoff water at a concentration of **slscr** (**slsci** and **slscr** are specified in the input file).
- by production in the profile: see Section I.3.4
- by artificial “creation” of solute when there is a constant potential top and/or bottom boundary condition for water flow (**itbc=1** or **ibbc=1**): the solute concentration at these boundaries is kept constant and in order to achieve this solute may be “created”. At the top boundary the solute concentration is held at the specified initial value (**csl(0)**), while for the bottom boundary it is specified separately in the input file as **csl(n)**.

3.4 Source/sink terms

The source/sink term ϕ in Eq. (50) contains four possible components, solute uptake by the vegetation, first-order decay of dissolved solutes, first-order decay of adsorbed solutes, and solute production (Kool and van Genuchten, 1991):

$$\phi = -\phi_{cr} - \lambda_1 \theta c - \lambda_2 \rho s + \phi_p \quad (64)$$

where

- ϕ_{cr} = solute uptake by the vegetation [μmol/cm³/h or μg/cm³/h]
- λ_1 = first-order decay coefficient for dissolved phase [1/h] ($-\lambda_1 = \mathbf{alpha(i)}$)
- λ_2 = first-order decay coefficient for adsorbed phase [1/h] ($-\lambda_2 = \mathbf{beta(i)}$)
- ϕ_p = solute production in the profile [μmol/cm³/h or μg/cm³/h]

Plant uptake of solute is assumed to take place only by mass flow. A proportionality factor **slupf** (0-1) is used to allow for partial or no uptake of certain solutes. The term ϕ_{cri} , for each layer is, therefore, given as:

$$\phi_{cri} = T_i c_i \text{ slupf} \quad (65)$$

where T_i is the rate of root water uptake in layer i and c_i is the solute concentration in water. Water uptake is discussed in Section I.4.3.

Solute production in the profile (through the ϕ_p term in Eq. 64) can be given as a function of depth and time in the input file. The user can define:

- a depth function (**idepth=0** or **idepth=1**) multiplied by a time function (**itime=0** or **itime=1**),
or
- a matrix of production with time and depth (**idepth=2**).

The depth and time functions define a production rate relative to a given maximum production rate (per unit depth) (**slpmax**). For the depth function, an exponential function (**idepth=0**) of the form $f = \exp(-x/\text{slxc})$ can be used, or depth-production pairs can be specified (**idepth=1**). As SWIMv2.1 uses these depth functions as integrated with depth, the depth-production pairs must be given as the cumulative values with depth. A cycle of solute production can also be specified (through **scycle**). For further details see Section I.4.1 and the examples in Section II.1.3, where root growth is specified in the same way. Solute production does not occur above and below the upper (**slpc1**) and lower (**slpc2**) cutoff potentials.

4. EVAPOTRANSPIRATION

4.1 General description

As described in Section I.1.3, soil evaporation and plant transpiration are treated as sink terms in the Richards' equation (Eq. 5). This Chapter describes how these sink terms are calculated and what assumptions are involved.

In SWIMv2.1 evaporation and transpiration rates are determined by both the evaporative demand placed on the system and by the soil's ability to supply water to meet this demand. Potential evapotranspiration (PET) reflects the demand and needs to be specified as input to the model. Common approaches that have been used to obtain PET values are pan evaporation with or without a crop correction factor, the Penman-Monteith model, and the Priestley-Taylor model (Rosenberg *et al.*, 1983). In SWIMv2.1's treatment of plant water uptake (Section I.4.3), the leaf or stomatal resistance and the aerodynamic resistance to transpiration are not treated explicitly. The demand is, therefore, expressed through the xylem potential. The effects of these two resistance factors are assumed to be incorporated in the specified PET, and the user needs to ensure that the "correct" PET is used for the application at hand.

SWIMv2.1 allows a flexible time scale for specifying PET by working from a record of cumulative potential evapotranspiration with time, and by using linear interpolation to obtain the values for the time steps used by SWIMv2.1. PET can thus be given on an hourly scale, e.g. to study diurnal patterns, or on a weekly, monthly, or longer time scale. Of course, while PET is fixed at the rate(s) specified in the input file, the actual water extraction will change in response to soil water status (soil's ability to supply water).

SWIMv2.1 allows PET to be intercepted by up to four vegetation types simultaneously. This enables one to simulate single crops, intercropping or mixed species (e.g. trees and grasses). Each vegetation type has certain characteristics that determine its water extraction pattern. These characteristics are, however, assumed to be fixed and known in advance. During a simulation run there is no feedback to the plant regarding its growth. SWIMv2.1 is not a plant growth model and it uses the imposed evaporative demand (PET) purely as a way to define the sink term in the Richards' equation. The description of plant water uptake is, therefore, less precise and more empirical than that of movement of water in the soil. For a more realistic simulation of plant water uptake, use SWIMv2.1 inside the APSIM framework (see Introduction).

When running SWIMv2.1 a fraction of the total PET is assigned to each vegetation type (*j*), with any left over being used for soil evaporation. The total percentage of PET intercepted by the vegetation can be larger than 100%, in which case nothing is left for soil evaporation. The fraction of PET intercepted by a vegetation type is a function of time and is specified in the input file. SWIMv2.1 can simulate sigmoidal "growth" with time (**igrow(j)=0**) or the user can specify time-"growth" pairs (**igrow(j)=1**). In the last case SWIMv2.1 uses linear interpolation to determine the interception fraction for a specific time. As explained above, this is not real plant "growth", but only represents the fractional interception of PET of a vegetation type. The equation describing the sigmoid relative "growth" curve has the following form:

$$f = 1 / (1 + \exp(a_1 - b_1 t)) \quad (66)$$

where t is the time and a_1 and b_1 are constants. The function f is multiplied by the maximum fraction of PET (**fevmax(j)**) to obtain the fraction of PET intercepted at time t . Equation (66) can represent both growth and decay, depending on the choice of a_1 and b_1 (see Fig. 7). In SWIMv2.1 it is also possible to define a sequence of growth followed by decay, or vice versa. This is achieved by using a second function of the same form as Eq. (66), but with two different constants (a_2 and b_2). The four constants (a_1 , b_1 , a_2 , and b_2) are calculated by SWIMv2.1 from four user defined points ((**f1,t1**) and (**f2,t2**) for the first function and (**f3,t3**) and (**f4,t4**) for the second function). A cycling time can also be imposed (**vcycle(j)**). In that case growth and decay alternate with a total cycle time of **vcycle(j)** hours.

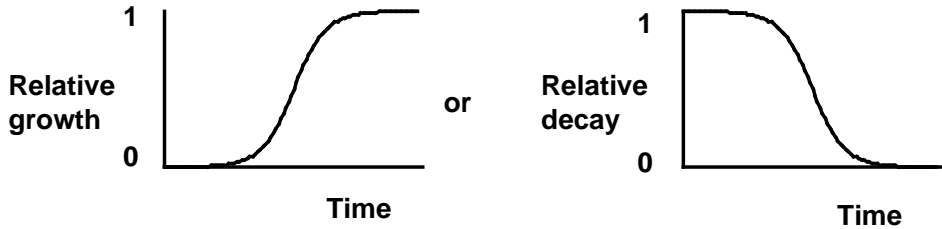


Figure 7: Sigmoid relative growth/decay functions.

In SWIMv2.1 water uptake by the roots is equated to transpiration, i.e. there is no storage of water in the plant. In addition to PET and the interception fractions, root distributions as functions of depth and time need to be specified. These, together with the root radius (**rad**) and the root conductance (**groot**), affect the supply rate of the soil (see Section I.4.3). SWIMv2.1 has various options for the input of the root distributions. The approach is to, for each vegetation j , multiply a maximum root length density (**rldmax(j)**) with a depth function and a time function that each express the root length distribution relative to this maximum. For the depth function, an exponential function of the form $f = \exp(-x/\mathbf{xc}(j))$ can be used (**iroot(j)=0**) or depth-“growth” pairs can be specified (**iroot(j)=1**). Because SWIMv2.1 uses an integrated depth function with depth, the depth-“growth” pairs must be given as the cumulative values with depth. If **iroot(j)** is equal to 0 or 1, then the time function is the same as that used for the interception of PET (**igrow(j)=0** or **igrow(j)=1**). Alternatively, a matrix of relative root length density with depth and time can be specified (**iroot(j)=2**). SWIMv2.1 interpolates first in time and then in depth. The depth component of this matrix must again be specified as cumulative values with depth. If this option is chosen, the PET interception fraction is still given by **igrow(0)** or **igrow(1)**. Interception and root length density are then not linked. See Example 1.2 in Section II.1.3 for examples of these root “growth” functions. Some experimentally determined, typical root distributions are given by Taylor and Klepper (1973, 1975), Robertson *et al.* (1980), and Ball-Coelho *et al.* (1992).

4.2 Soil evaporation

The procedure for calculating soil evaporation is based on that of Campbell (1985). The soil evaporation rate is calculated as a fraction of the potential evaporation, which is defined as the evaporation that would occur if there was a continual supply of water to the surface, such as occurs in saturated soil. As long as the conductive properties of the soil are not limiting, the actual evaporation is equal to the potential evaporation.

Evaporation at the soil surface is given by:

$$E = \frac{\rho_{vs} - \rho_{va}}{r_v} \quad (67)$$

where

E = evaporation rate per unit area [cm/h]

ρ_{vs} = vapour density at the soil surface [kg/cm³]

ρ_{va} = atmospheric vapour density (i.e. of air above soil surface) [kg/cm³]

r_v = boundary layer and aerodynamic resistance [(kg/m²)/(cm/h)]

At the surface of a saturated soil, we have

$$E_p = \frac{\rho'_{vs} - \rho_{va}}{r_v} \quad (68)$$

where

ρ'_{vs} = saturated vapour density at the soil surface [kg/cm³]

E_p = potential evaporation rate [cm/h].

Combining Eq. (67) and (68) gives

$$\frac{E}{E_p} = \frac{\rho_{vs} - \rho_{va}}{\rho'_{vs} - \rho_{va}} \quad (69)$$

For an isothermal system the vapour density is related to the relative humidity h by

$$\rho_v = \rho'_v h \quad (70)$$

where ρ'_v is the saturated vapour density at the particular temperature. For a saturated soil $h=1$, so that $\rho_{vs} = \rho'_v$. Combining Eq. (69) and (70) then leads to

$$\frac{E}{E_p} = \frac{\rho'_v h_s - \rho'_v h_a}{\rho'_v - \rho'_v h_a} \quad (71)$$

where

h_s = relative humidity at the soil surface [-]

h_a = relative humidity of the atmosphere above the soil [-] (**hair**)

This simplifies to the equation that is central to SWIMv2.1's surface evaporation routine (Campbell, 1985):

$$E = E_p \frac{h_s - h_a}{1 - h_a} \quad (72)$$

The relative humidity of the atmosphere h_a (**hair**) is specified in the SWIMv2.1 input file. In SWIMv1 it was equal to 0.5. In practice, the calculations are not very sensitive to the choice of h_a .

The relative humidity, h , is a function of the soil matric potential:

$$h = \exp(M_w \psi_t g / RT) \quad (73)$$

- M_w = mass of one mole of water (0.01802) [kg/mol]
 ψ_t = soil total potential [cm]
 g = gravitational constant ($9.81 * 10^2$) [cm/s²]
 R = gas constant ($8.3143 * 10^4$) [kg cm²/s²/mol /K]
 T = absolute temperature [K]

The value for h_s is evaluated from ψ_t at the surface, which in turn is obtained from the general analysis of flow in the soil (see Section I.1.2). If no solutes are present, ψ_t is equal to the matric potential; otherwise, ψ_t also includes the osmotic potential (see Section I.4.4). It follows from Eq. (72) and (73) that if $\psi_t = 0$ then E is equal to E_p , e.g. when the soil is saturated and the osmotic potential can be ignored (no solutes). When the soil dries out and water cannot be supplied fast enough, $E < E_p$. As explained in Section I.4.1, the potential evaporation, E_p , is the fraction of the user-provided potential evapotranspiration that is left over after interception by the various vegetation types.

4.3 Plant water uptake

The transpiration rate is calculated using a method based on that of Campbell (1985). This method treats the soil-plant-atmosphere continuum as a resistance network. While Campbell (1985) treats the system as a whole, SWIMv2.1 assumes that the demand for water is expressed through the xylem potential (ψ_x), and that the stomatal and aerodynamic resistance effects are incorporated in the specified PET. In addition, the axial resistance in the xylem is assumed negligible compared with the other resistances. The resistances that are considered by SWIMv2.1 are, therefore, the soil resistance (R_s) and the root endodermis resistance (R_r) (Fig. 8). Water thus moves from the soil to the xylem through a soil and root resistance. By analogy to Ohm's law the transpiration flow for a uniform soil layer i can be defined as

$$T_i = (\psi_{s0i} - \psi_x) / (R_{si} + R_{ri}) \quad (74)$$

where

- T_i = transpiration rate of layer i per unit area [cm³ water/cm² soil/h]
 ψ_{s0i} = soil matric potential layer i [cm water]
 ψ_x = xylem potential [cm water]
 R_{si} = soil resistance of layer i [h cm² soil/cm² water]
 R_{ri} = root resistance of layer i [h cm² soil/cm² water]

In order to calculate the root water uptake rate for each soil layer using Eq. (74), it is necessary to determine the soil and root resistances of the various layers, and then find the balance between the xylem potential and the the potential transpiration (T_p). The soil resistance is calculated assuming steady-state radial flow to the roots, while the root resistance is obtained from a resistance per unit length of root and the root length density of each layer. The various steps are discussed in more detail below.

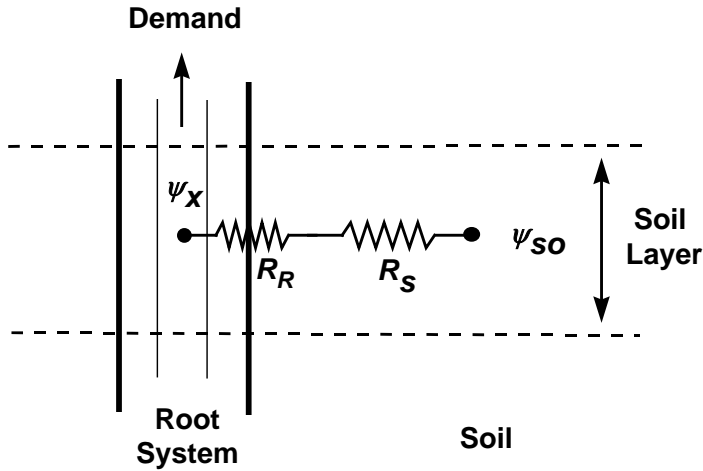


Figure 8: Analog showing resistances and potentials taken into account in the simulation of plant water uptake.

Soil resistance

The soil resistance of layer i , R_{si} , is determined by the soil hydraulic conductivity, root length density, and water uptake rate (Gardner, 1960; Cowan, 1965; Campbell, 1985). Following Campbell (1985), SWIMv2.1 uses the analysis of Cowan (1965) for water uptake by a single root to obtain this resistance term. The differential equation for water uptake by a single, cylindrical root surrounded by a cylinder of homogeneous soil is given as

$$\frac{Q}{A} = -K \frac{d\psi}{dr} \quad (75)$$

and

$$A = 2\pi rl \quad (76)$$

where

- Q = rate of water uptake by the root [cm^3 water/h]
- K = soil hydraulic conductivity [cm^2 water/cm soil/h]
- ψ = matric potential [cm water]
- r = radial distance from the root axis [cm]
- A = area of water flow [cm^2 l]
- l = length of root [cm]

The soil hydraulic conductivity K in Eq. (75) is the same as that in Eq. (5) and depends on ψ as specified in Section I.2.2. If vapour flow is included (**ivap=1**), it is added to the hydraulic conductivity (see Section I.2.4). In the example here we assume a Brooks-Corey type relation

$$K = K_s \left(\frac{\psi_e}{\psi} \right)^n \quad (77)$$

where

K_s = saturated conductivity [cm^2 water/cm soil/h]

ψ_e = air entry potential [cm]

n = constant depending on soil type [-]

For steady state flow (Q is constant with r), combining Eq. (75) and (77) and integrating from the outside of the soil cylinder r_{s0} (where the potential is ψ_{s0} and the conductivity K_{s0}) to the root surface at r_r (where the potential is ψ_r and the conductivity K_r), gives

$$\frac{Q}{2\pi l} \ln \frac{r_r}{r_{s0}} = \frac{K_{s0} \psi_{s0} - K_r \psi_r}{1-n} \quad (78)$$

The root radius r_r is an input parameter in the input file of SWIMv2.1 (**rad**). For sugarcane Ball-Coelho *et al.* (1992) measured root radia in the range of 0.005 - 0.11 cm with an average of 0.024 cm. Values for other crops can be found in e.g. Huck *et al.* (1970), Föhse *et al.* (1991), and Eghball and Maranville (1993). SWIMv1 used a value of 0.1 cm.

The distance r_{s0} corresponds to a point midway between the roots. Treating each root individually would, however, lead to a geometrically complicated system involving many differential equations. A macroscopic approach (Hillel, 1980) is, therefore, taken, in which the root system in each soil layer is treated as a diffuse sink. This is achieved by working with root length densities (L_i). Only horizontal flow is taken into account, so that the root water uptake in each layer is treated independently and the gravity component can be ignored. The distance r_{s0i} of a layer can be expressed in terms of the root length density of that layer (Gardner, 1960; Cowan, 1965; Campbell, 1985) according to

$$r_{s0i} = (\pi L_i)^{-1/2} \quad (79)$$

For each soil layer i , the water uptake rate, Q_i , per unit length of root can be related to the root length density, the thickness of the layer and the transpiration rate T_i ; thus providing a link between Eq. (74) and (75)

$$\frac{Q_i}{l_i} = \frac{T_i}{L_i \Delta x_i} \quad (80)$$

where

l_i = root length in layer i [cm root]

L_i = root length density of layer i [cm root/cm³ soil]

Δx_i = thickness of layer i [cm soil]

Substituting Eq. (79) and (80) into Eq. (78) yields

$$T_i = (K_{s0i} \psi_{s0i} - K_{ri} \psi_{ri}) / B_i \quad (81)$$

where

$$B_i = (1-n) \ln(\pi r_r^2 L_i) / (4\pi L_i \Delta x_i) \quad (82)$$

Since the analysis is only approximate, SWIMv2.1 assumes that Eq. (77) with $n = 2$ can be used for any form of conductivity function (Section I.2.2).

At steady state (compare Eq. 74)

$$R_{si} = (\psi_{s0i} - \psi_{ri}) / T_i \quad (83)$$

so that

$$R_{si} = B_i (\psi_{s0i} - \psi_{ri}) / (K_{s0i} \psi_{s0i} - K_{ri} \psi_{ri}) \quad (84)$$

Since B_i depends on rooting depth and root length density, R_{si} will be a function of these variables as well. SWIMv2.1 assumes $K_{ri} \approx K_{s0i}$ so that Eq. (85) simplifies to

$$R_{si} = B_i / K_{si} \quad (85)$$

Therefore, if the root radius, the root length density, the layer thickness, soil matric potential and conductivity are known, the soil resistance can be calculated.

Root resistance

The root resistance of layer i , R_{ri} , is inversely proportional to the root length density in layer i

$$R_{ri} = 1 / (g_r L_i \Delta x_i) \quad (86)$$

where

- g_r = root conductance (**groot**) [cm^2 water/h/cm root]
- L_i = root length density of layer i [cm root/ cm^3 soil]
- Δx_i = thickness of layer i [cm soil]

Values given by Bristow *et al.* (1984) for the resistance of sunflower roots per unit length translate into a g_r of $1.4 \cdot 10^{-7} \text{ cm}^2$ water/h/cm root. Values for other crops may be found in e.g. Herkelrath *et al.* (1977a,b; wheat), McAneny and Judd (1983; kiwifruit), Nobel and Cui (1992; succulents).

Balance between xylem potential and potential transpiration

The total transpiration is given by

$$T = \sum_i T_i = \sum_i \frac{\psi_{s0i}}{R_{si} + R_{ri}} - \psi_x \sum_i \frac{1}{R_{si} + R_{ri}} = \sum_i \frac{\psi_{s0i} - \psi_x}{R_{si} + R_{ri}} \quad (87)$$

SWIMv2.1 first determines the maximum soil supply, T_{max} , by setting ψ_x = minimum xylem potential (**psimin(i)**). This maximum supply is compared with the potential transpiration T_p . If $T_{max} < T_p$, then the actual transpiration, T_a , is equal to the maximum soil supply T_{max} . If $T_{max} > T_p$, then T_a is set equal to T_p and Eq. (87) is used to solve for ψ_x . While Eq. (87) with $T = T_p$ gives a solution for ψ_x directly, SWIMv2.1 uses an iteration procedure where layers with $\psi_x > \psi_{s0i}$ are excluded from the summations in Eq. (87), as this would lead to flow of water from the roots to the soil.

4.4 Osmotic effects

When solutes are present in the system, the transport of water through semipermeable membranes is affected by the presence of an osmotic potential. SWIMv2.1 takes this osmotic potential (ψ_o) into account at the soil-root boundary and at the soil surface boundary. The osmotic potential is given by (Campbell, 1985)

$$\psi_o = -\nu c \chi R T / (g \rho_w) \quad (88)$$

where

ψ_o	= osmotic potential [cm]
ν	= number of particles in solution/molecule of solute [-]
c	= solute concentration [$\mu\text{mol}/\text{cm}^3$]
χ	= osmotic coefficient [-]
R	= gas constant ($8.3143 * 10^{-2}$) [$\text{kg cm}^2/\text{s}^2/\mu\text{mol}/\text{K}$]
T	= absolute temperature [K]
g	= gravitational constant ($9.8 * 10^2$) [cm/s^2]
ρ_w	= density of water ($1.0 * 10^{-3}$) [kg/cm^3]

Robinson and Stokes (1965, App. 8.9 and 8.10) give values of the osmotic coefficient, χ , for common solutes. It is approximately equal to unity for dilute solutions. SWIMv2.1 lumps the effects of ν , χ , R , T , g , and ρ_w into a proportionality constant **slos**, which needs to be specified in the input file. As SWIMv2.1 allows c to have different units than those given above, any unit conversion should be accounted for in **slos**. (see Example 1.4 in Section II.1.3). For programming convenience, the osmotic potential is included in the soil matric potential (e.g., ψ_{soi} in Eq. 87). Because SWIMv2.1 solves the solute transport equation after it solves the water flow and uptake, the value used for ψ_o is the value of the previous time step.

4.5 Changes from SWIMv1

- In SWIMv1 the interception fraction of PET and root length density were defined using the functions **iroot(0)** and **igrow(0)**.
- In SWIMv1 the analysis for transpiration used Eq. (84) instead of Eq. (85).
- In SWIMv1 the uptake by the roots was calculated before the solution of the flow equation where it appeared as a constant sink term during the solution. SWIMv2.1 includes the calculations in the iterative solution of the flow equation, although it is fixed at a constant value when it is changing less than the value of **errex** specified in the input file, so that the flow equation can be solved efficiently to a high precision to give good mass balance.
- As solutes were not included in SWIMv1, the effect of osmotic potential on evaporation and root water uptake was not considered.
- The parameters **hair**, **rad**, and **groot** need to be specified in the input file for SWIMv2.1, whereas they were “hard-wired” in SWIMv1 (0.5 , 0.1 cm, $1.4 * 10^{-7}$ $\text{cm}^2/\text{h}/\text{cm}$, respectively).

5. PROCESSES AT THE SOIL SURFACE

5.1 Rainfall

Rainfall and/or irrigation are given as inputs to SWIMv2.1 in the form of a cumulative record with time. Both are assumed to fall at a constant rate during the period between two input points. For the water balance calculations, SWIMv2.1 uses linear interpolation to calculate how much rainfall or irrigation fell during each time step, dt .

SWIMv2.1 also uses the rainfall and/or irrigation record to calculate the rainfall intensity, I , and the cumulative kinetic energy. This information is used in the calculations of surface conductance and surface roughness decline (see Sections I.5.2 and I.5.3). A logarithmic equation relates the kinetic energy per unit precipitation to the intensity of the precipitation (e.g., Hudson, 1981; Moore, 1981):

$$KE = a + b \ln(I) \quad (89)$$

where

KE = kinetic energy per unit surface area per unit precipitation [$J/cm^2/cm$ rain]
 I = rainfall intensity [cm/h]
 a, b = constants

In these units, the equation given by Wischmeier and Smith (1958) translates into

$$KE = 0.02062 + 0.00379139 \ln(I) \quad (90)$$

and that of Zanchi and Torri (1981) into

$$KE = 0.002106 + 0.0048858129 \ln(I) \quad (91)$$

In SWIMv2.1 the kinetic energy is taken relative to that of precipitation that falls with an intensity of $I_r = 2.5$ cm/h. For rainfall with this intensity Eq. (89) becomes

$$KE_r = a + b \ln(I_r) \quad (92)$$

Combining Eq. (89) and (92) and rearranging gives

$$r_{KE} = KE / KE_r = 1 + (b / KE_r) \ln(I/I_r) = 1 + E_{ff} \ln(I/I_r) \quad (93)$$

where E_{ff} is called the effectiveness parameter (**effpar**) [-]. r_{KE} is a measure of the energy in an amount of precipitation of intensity I compared with that of the same amount of precipitation of intensity I_r .

Based on Eq. (90) and (91) E_{ff} should be approximately 0.157 - 0.191. In the reference manual of SWIMv1 (Ross, 1990b) a value of 0.184 was suggested. Note that when the equations are written with $^{10}\log$ instead of \ln , the magnitude of E_{ff} changes. The effectiveness parameter E_{ff} should only be used when realistic intensity information is given. If daily precipitation is used it may be best to set $E_{ff} = 0$, so that all precipitation is equally effective in reducing the surface conductance and surface roughness (see Sections I.5.2 and I.5.3).

SWIMv2.1 uses Eq. (93) to convert the actual precipitation amounts (*rain*) of given intensity *I* to their equivalent 2.5 cm/h (I_r) precipitation amounts (*eqrain*) according to:

$$eqrain = r_{KE} * rain \quad (94)$$

where *rain* and *eqrain* are both in [cm]. SWIMv2.1 keeps a cumulative record (*cegrain*) of *eqrain* since the start of the simulation run or since the last cultivation (see Section I.5.4), in order to calculate the decline in surface conductance and roughness due to rainfall (see Section I.5.2 and I.5.3). Note that r_{KE} in Eq. (93) could become negative for very small values of *I* (e.g., <0.0109 cm/h if $E_{ff} = 0.184$). If this happens, SWIMv2.1 resets r_{KE} to zero.

5.2 Surface sealing

The option of including a surface conductance function (**itbc=2**, see Section I.1.3) allows SWIMv2.1 to deal with sealing and crusting soils. Rather than simulating a surface layer of variable thickness, the seal is represented by an infinitely thin “membrane” that is characterised by a conductance *G* (see Fig. 9). The water flux through the seal is equal to this surface conductance multiplied by the matric potential difference across it. The seal is only present when there is ponded water, and it does not affect soil evaporation.

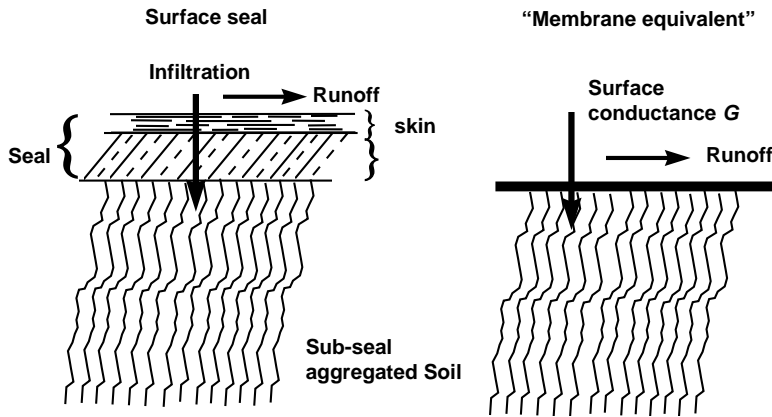


Figure 9: Simulation of a seal in SWIMv2

SWIMv2.1 allows time dependence of the seal properties by letting the surface conductance decrease exponentially with cumulative rainfall energy (e.g., Moore, 1981)

$$G = G_{min} + (G_{initial} - G_{min}) \exp(-E/E_{cs}) \quad (95)$$

where

G = conductance of the seal [1/h]

G_{min} = minimum seal conductance [1/h] (**g0**)

$G_{initial}$ = initial seal conductance [1/h] (**g1**)

E = cumulative rainfall energy per unit surface area [J/cm^2]

E_{cs} = energy in an amount of rain equal to the specified conductance precipitation constant (**grc**) falling at 2.5 cm/h [J/cm^2]

Because SWIMv2.1 converts actual amounts of rain (*rain*) into equivalent 2.5 cm/h rain (*cegrain*, Section I.5.1) we have

$$\begin{cases} E &= cegrain * KE_r \\ E_{cs} &= \mathbf{grc} * KE_r \end{cases} \quad (96)$$

so that

$$E / E_{cs} = crain / \mathbf{grc} \quad (97)$$

The conductance precipitation constant (**grc**), an input parameter, thus determines how fast G decreases. It has units of [cm]. Equations (94) and (96) specify that G falls 63% of the way ($\exp(-1) = 0.37$) after an amount of rainfall that has the equivalent cumulative energy of a storm of **grc** cm which falls at a rate of 2.5 cm/h. SWIMv2.1 calculates the rainfall intensities and cumulative kinetic energy at the beginning of its run (see Section I.5.1). G can be reset to $G_{initial}$ through cultivation (see Section I.5.4). SWIMv2.1 is currently set up so that G equals G_{min} at the beginning of the simulation run (time = **t0**), i.e. the subscript *initial* only refers to the situation immediately after cultivation. With a cultivation at **t0**, the simulation run can start with $G_{initial}$.

Ross (1990b, SWIMv1 Reference Manual) presents a simple way to estimate the conductance of a crust by dividing the saturated conductivity of the crust by its thickness. E.g., for a crust thickness 0.5 cm, and a saturated hydraulic conductivity of 0.2 cm/h, the conductance is $(0.2 \text{ cm/h}) / (0.5 \text{ cm}) = 0.4 \text{ /h}$. Other methods can be found in e.g. Moore (1981), Baumhardt *et al.* (1990), Silburn and Foley (1994), and Bridge and Silburn (1995).

5.3 Surface runoff

Runoff in SWIMv2.1 is based on the assumption that the soil has a certain surface roughness, which can detain water and prevent it from running off. The amount of surface water storage is related but usually not equal to the height of the roughness elements. SWIMv2.1 defines the parameter h_0 as the depth of water on the surface ($\text{cm}^3 \text{ water/cm}^2 \text{ surface area}$) when runoff just starts (see Fig. 10 for a simplified schematic). As only part of the surface may be covered, h_0 will usually be less than the height of the roughness elements. As indicated in Section I.1.3 the SWIMv2.1 user can choose to use a simple power-law function that specifies the net runoff rate (options **isbc=2** and **isbc=3**). The impact of rainfall on surface roughness is discussed first.

Surface roughness

The depth of water detained above a soil surface changes with time due to the impact of rain that causes a decrease in the height of surface roughness elements. The surface storage is, therefore, allowed to decrease with cumulative rainfall energy in the same fashion as the surface conductance:

$$h_0 = h_{0min} + (h_{0initial} - h_{0min}) \exp(-E/E_{cr}) \quad (98)$$

where

h_{0min} = minimum surface storage [cm] (**hm0**)

$h_{0initial}$ = initial surface storage [cm] (**hm1**)

- E = cumulative rainfall energy per unit area [J/m^2]
 E_{cr} = energy in an amount of rain equal to the given storage precipitation constant (**hrc**) falling at 2.5 cm/h [J/m^2]

As with surface conductance, h_0 can be reset to $h_{0initial}$ through cultivation (see Section I.5.4). The value of h_0 at the beginning of the simulation is equal to h_{0min} , unless a cultivation is performed at time $t=t_0$, in which case it is equal to $h_{0initial}$. Moore and Larson (1979) present a method to estimate micro-relief surface storage.

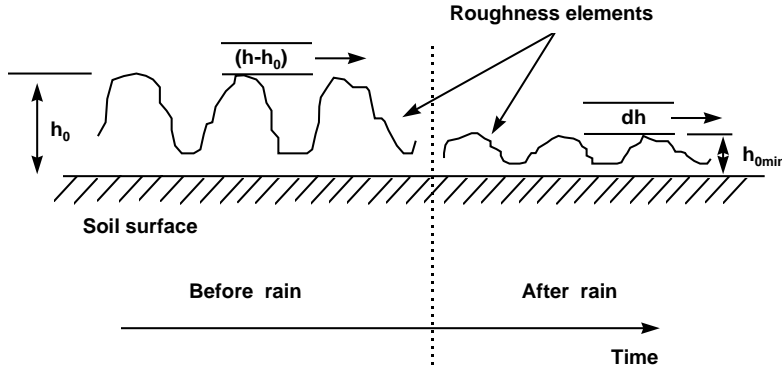


Figure 10: Runoff, surface roughness and decline with time (while strictly not correct, for simplicity h_0 is here assumed equal to surface roughness

Simple power-law runoff function

The simple power-law runoff function (**isbc=2 or 3**) is given by

$$R = \begin{cases} 0 & , h \leq h_0 \\ a(h - h_0)^b & , h > h_0 \end{cases} \quad (99)$$

where

- R = net runoff rate (i.e. rate “off” - rate “on” from upslope [cm/h])
 a = empirical constant (**roff0**)
 b = empirical constant (**roff1**)

It must be remembered that this net runoff rate is much smaller than the overland flow rate itself.

Equation (99) has a form similar to that resulting from applying the Manning equation for the flow velocity in open channels (e.g. Hudson, 1981)

$$v = \frac{1}{n} r^{2/3} \sqrt{s} \quad (100)$$

where

- v = mean runoff flow velocity [cm/s]
 r = hydraulic radius [cm]
 s = slope gradient [cm/cm]
 n = Manning’s roughness coefficient (**roff0**)

As the cross-section of overland flow is very wide and shallow, the hydraulic radius can be assumed equivalent to the depth ($h-h_0$) (Emmett, 1978). For turbulent flow with a steady-state depth (constant down the slope) runoff is governed by the continuity equation

$$q = (h - h_0)v \quad (101)$$

where q is the runoff at a point [cm^2/s] due to all upslope runoff.

Combining Eq. (100) and (101) gives (Emmett, 1978)

$$q = \frac{1}{n} (h - h_0)^{5/3} \sqrt{s} \quad (102)$$

In equations for laminar overland flow, q is proportional to $(h-h_0)^3$ (Emmett, 1978). Because surface runoff is probably a mixture of turbulent and laminar flow and to remove the dependence of Manning's n on units of length, it is convenient to use an exponent of 2. Also, because SWIMv2.1 works with a net runoff rate (see above), the right-hand side of Eq. (102) needs to be divided by the slope length, L_0 [cm]. With a conversion from seconds to hours (*3600), the surface runoff equation based on the Manning equation becomes

$$R = \begin{cases} 0 & , h \leq h_0 \\ 3600 \frac{1}{nL_0} (h - h_0)^2 \sqrt{s} & , h > h_0 \end{cases} \quad (103)$$

In Eq. (103) Manning's n has the units of [s]. The similarities between Eq. (103) and Eq. (99) (simple power-law function) are obvious. Values for Manning's n can be obtained from Hudson (1981). For clean surfaces n is approximately 0.016 and for more irregular surfaces it can increase to 0.030, or even 0.150 in the case of vegetated surfaces. Strictly speaking n changes with time if the surface roughness changes. Hence the parameter a in Eq. (99) should then change as well, but currently SWIMv2.1 only allows h_0 to change.

5.4 Cultivation

SWIMv2.1 allows for regular cultivation (cyclical) or cultivation at specified times. Cultivation can mean one or more of the following:

- the surface is disturbed, so that surface conductance (Section I.5.2) and surface storage (Section I.5.3) are reset to their initial values,
- solute is added to the surface; the amount that will dissolve into the infiltrating water and into runoff is specified by **slsci** and **slscr**, respectively (Section I.3.3)

Cultivation is necessary at time=**t0** if the simulation needs to start with the initial values for surface conductance and surface storage. In the case of cycling, $t=\mathbf{t0}$ is the start of the cycle. Any given times will then be repeated every cycle. Note that cultivation does not have any effect on soil hydraulic properties, except for the surface (crust) conductance and roughness.

Cultivation can also be used to obtain simulation output at selected times, rather than or in addition to the regular output intervals. It can also be used to adjust the time step such that the equations are solved to specific points in time (the specified "cultivation" times).

6. TECHNICAL DETAILS

Iteration to solve Richards' Equation

The nonlinear discretised equation (Eq. 7) arising at each time step in the solution of Richards' equation is solved using the Newton-Raphson method (see e.g. Campbell, 1985). If a solution cannot be found to the requested accuracy in a reasonable number of iterations the time step is halved and, provided the new time step is above the minimum set (**dtmin**) and also above 0.01 of the initial step, the procedure is repeated. If a solution is still not found the program exits after printing an error message. It may still be possible to obtain a solution by altering the grid spacing or the time step (either by altering **dtmin** or **dw**). The accuracy required is set with **ersoil** and **ernode**, which specify respectively the allowable flux balance error (in cm/h) in the soil profile as a whole and at each node for the time step. Values of 0.000001 are usually satisfactory, but raising these may sometimes help in obtaining a solution. The error **errex** is the relative fraction of the plant water uptake rate at which the rate will become fixed, i.e. no longer changing from iteration to iteration; it should not be set too small for efficiency (0.01 is reasonable). During iteration it is sometimes necessary to limit the size of changes in the transformed variable p as discussed by Ross (1990a). The parameters **dppl** (increasing p) and **dpnl** (decreasing p) achieve this; values of 2 and 1 respectively are generally satisfactory.

Surface conductance and evaporation

When a surface conductance due to soil sealing (**itbc=2**) has been specified rather than an infinite conductance (**itbc=0**, zero resistance to flow), infiltration is affected whenever the surface is ponded. However, evaporation occurs unimpeded from the soil surface under the (infinitely thin) seal whether the surface is ponded or not.

Layer interfaces

Nodes can be positioned on layer interfaces simply by repeating the depth with a different property set associated (see Fig. 11). The output will give the same matric potential and flux for the two nodes, since these are continuous across layer interfaces, but will give different water contents. Similarly solute concentrations in solution and fluxes will be the same, but total solute concentrations will differ since these depend upon water content and soil properties.

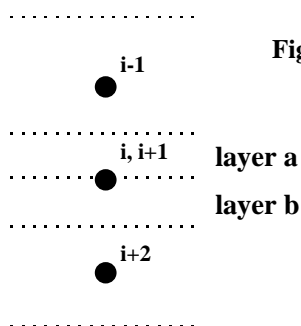


Figure 11: Discretisation in space when two nodes are specified with the same depth; layer a and b have the same matric potential and solute concentration in solution, but can differ in water content, hydraulic conductivity, and total solute concentration if the hydraulic and solute properties of the nodes are different.

Iteration to solve the advection-dispersion equation

When the exchange isotherm is not present (**exco**=0) or is linear (**fip**(**i**)=1), the solute transport equations are linear and are solved without iteration; otherwise the Newton-Raphson method is used. Since only the coefficients depending on the exchange isotherm change, for efficiency only these are updated each iteration. The allowable convergence error for solute concentration is given by **slcerr**. The recommended value is 0.000001.

Spatial weighting for the advection-dispersion and Richards' equations

The steady-state form of the advection-dispersion equation (cf. Eq. 50) is given as

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \quad (104)$$

where

D = combined dispersion and diffusion coefficient [cm^2/h]

v = pore water velocity = q/θ [cm/h]

Spatially discretising this equation using central differences we obtain for node i

$$\begin{aligned} \frac{dc_i}{dt} &= D \left(\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} \right) - v \left(\frac{c_{i+1} - c_{i-1}}{2\Delta x} \right) \\ &= \left(\frac{D}{\Delta x^2} + \frac{v}{2\Delta x} \right) c_{i-1} - \frac{2D}{\Delta x^2} c_i + \left(\frac{D}{\Delta x^2} - \frac{v}{2\Delta x} \right) c_{i+1} \end{aligned} \quad (105)$$

The solution of the differential equations leads to concentrations that oscillate in time if the coefficient of c_{i-1} or c_{i+1} is negative, i.e. if the local Peclet number $Pe = |v|\Delta x/D$ is greater than 2. The oscillations can be suppressed by using an upstream weighting for the first order spatial derivative, giving

$$\begin{aligned} \frac{dc_i}{dt} &= D \left(\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} \right) - v \left(w_1 \frac{c_i - c_{i-1}}{\Delta x} + w_2 \frac{c_{i+1} - c_i}{\Delta x} \right) \\ &= \left(\frac{D}{\Delta x^2} + \frac{w_1 v}{\Delta x} \right) c_{i-1} - \left[\frac{2D}{\Delta x^2} + \frac{(w_1 - w_2)v}{\Delta x} \right] c_i + \left(\frac{D}{\Delta x^2} - \frac{w_2 v}{\Delta x} \right) c_{i+1} \end{aligned} \quad (106)$$

where w_1 and w_2 are weighting factors and $w_1 + w_2 = 1$.

Then, when $Pe > 2$, we can choose $w_2 = D/v\Delta x$ for $v > 0$ and $w_1 = -D/v\Delta x$ for $v < 0$. This is effectively adding a numerical dispersion of $(w_1 - 0.5)v\Delta x$ for $v > 0$; if the coefficient D is assumed proportional to the velocity then this is equivalent to a dispersivity ε of $(w_1 - 0.5)\Delta x$ (compare Eq. (51) with $D_0 = 0$ and $n = 1$). The weighting is also effectively calculating an upstream weighted advective flux between nodes as $v(w_1 c_{i-1} + w_2 c_i)$. A similar weighting scheme can be used when D and v are not constant, applied to the flux between nodes according to the values of D and v there, but the treatment is then only approximate. A similar treatment applies for the Richards' equation (Eq. 7) where the gravity term is treated like the advective term in the above. In the equations for the weighting Kd is analogous to D , gdK/dp to v and p to c .

In SWIMv2, **slswt** and **swt** define the weighting used for the advective-dispersive and Richards equations, respectively (see Eq. (7), (14), (56), and (60)). A value from 0.5 to 1 is taken as defining w_1 . Any other value greater than -1 is taken as indicating that the scheme above is required. A value $-a$ (negative **swt** or **slswt**) less than -1 causes the Peclet number to be divided by a before applying the above scheme, i.e. central weighting is used until $Pe=2a$ and upstream weighting $w_2=aD/v\Delta x$ ($v>0$) is then applied. This potentially allows some oscillation but will reduce smearing of fronts due to numerical dispersion. Effects of numerical dispersion are best studied by using finer grids - numerical dispersion is thereby reduced so that its contribution on coarser grids can be assessed.

Figure 12 below shows effects of numerical dispersion with different weighting factors when $D=0$. Water with a solute concentration of 1.0 was applied to a wet soil for 20 h at a constant rate of 1 cm/h (giving $v=2.5$ cm/h).

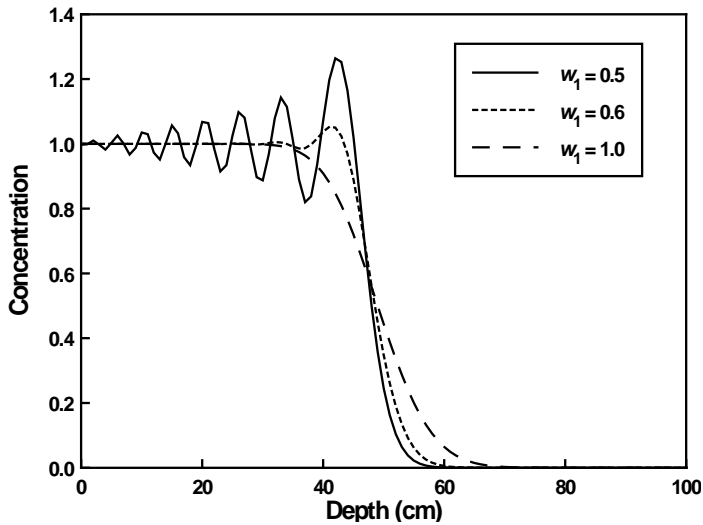


Figure 12: Effect of weighting factors on oscillation and numerical dispersion.

Figure 13 illustrates effects of weighting and grid spacing when $D=1$ cm²/h and other conditions are as above. With a grid spacing of 8 cm and **slswt**=0 there is considerable numerical dispersion, and with **slswt**=0.5 oscillations occur. With a grid spacing of 2 cm there are no oscillations (even though $Pe=5$) and with a further reduction of grid spacing to 1 cm identical results are obtained, indicating that no further improvement can be gained. More detailed discussions of numerical dispersion can be found in standard texts on numerical methods for advective problems (e.g. Pinder and Gray, 1977).

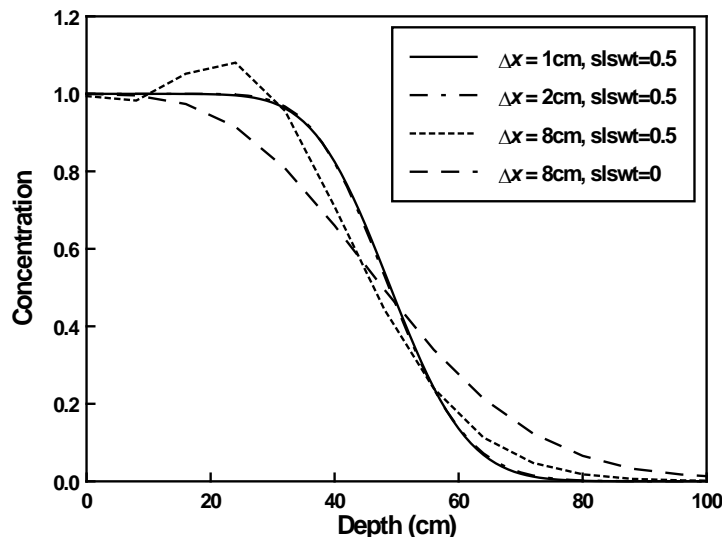


Figure 13: Effects of weighting and grid spacing on numerical dispersion.

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SWIMv2.1 User Manual

II - INSTRUCTIONS

1. USING SWIMv2.1

In order to use the SWIMv2.1 model to simulate water and solute transport, it is necessary to convert measured or estimated hydraulic properties into a form that the SWIMv2.1 program accepts. For this purpose the program HYPROPS is provided (see Section II.2). This program needs to be run first, as its output is used to prepare the SWIMv2.1 input file.

SWIMv2.1 has run successfully if the message “Stop - Program terminated” appears on the screen. The output of SWIMv2.1 consists of the output to the screen (console output) and a binary output file *filename.out*. The output to the screen can be redirected to a file by adding at the end of the running command “>*filename.con*” (see below). The binary *filename.out* file can be viewed using the program SWIMPLOT (see Section II.3) if an @ is used in the first line of the input file (version number) (see Section II.1.2). The *filename.out* file can also be converted to ASCII tables with the use of the program SWIMREAD (see Section II.4).

1.1 Running SWIMv2.1

To run SWIMv2.1 type the following command line at the DOS prompt:

```
swimev filename.in2 [filename.out /n /t /b /d /a /h /sfilename.fin /rfilename.fin >filename.con]
```

where *filename.in2* and *filename.out* are the names of the input and output files respectively, and:

/n	no console output
/t	time only console output
/b	brief console output
/d	detailed console output
/a	append the output to an existing output file <i>filename.out</i>
/h	start the output file <i>filename.out</i> with the header of the input file <i>filename.in2</i>
/sname	used with filename (' <i>filename.fin</i> ') immediately following the '/s'; This option saves the final state (matric potential profile, hysteresis state, and solute concentration profile) to the file ' <i>filename.fin</i> '.
/rname	used with filename (' <i>filename.fin</i> ') immediately following the '/r'; This option restores the initial state (matric potential profile, hysteresis state, and solute concentration profile) from the file ' <i>filename.fin</i> '.
> <i>filename.con</i>	MS-DOS command for redirection of screen output to the file <i>filename.con</i>

All arguments except *filename.in2* are optional. Multiple switches are possible, except that the switches /n, /t, /b, and /d are mutually exclusive. If you use two or more of these switches, then the last one in the list will be used. Otherwise, the order of the switches does not matter. Note that any existing file *filename.out* is overwritten unless switch /a is used. However, switch /h overrides switch /a if both switches are specified, so that the file *filename.out* is still overwritten.

Using no arguments other than *filename.in2* results in a run without output. If the switch /t is used, only the times of the output time steps (specified in input file, see Section II.1.2) are printed to the screen. If /b is used, information on the evaporation and transpiration rates and the water and solute balance components is printed to the screen at every output time step. The switch /d provides in addition information about the individual depth nodes (see Example 1.1, Section I.1.3). The switches do not affect the information given in the binary output file *filename.out*.

The switch /a causes the output to be appended to an existing output file (*filename.out*). It can be used to combine the output of a series of runs into one. The switch /h causes the output file to start with some details of the input file name and the first line of the input file (version number). This is purely for identification purposes. The switch /s allows one to save the final state of the simulation to the file '*filename.fin*'. It can then be used in a subsequent run (using /r and same file name) to restore this final state as the initial state of this second run. It then overrides the initial state specified in the input file of the second run. These switches can be useful if certain parameters that SWIMv2.1 does not allow to be varied during a run, need to be changed (e.g. change of type of cultivation and hence runoff and surface conductance parameters).

1.2 Preparing the input file for SWIMv2.1

The input file structure for SWIMv2.1 is given below using logical statements (*if..then..else..endif* and *do i=1,n .. end do*). The **bold** parameters need to be provided by the user, as specified by the instructions. Not all bold parameters need to be provided. The logical statements (in *italic* print) cause the input file to have a different structure when different choices are made for e.g. the boundary conditions, the inclusion of solutes and hysteresis, etc. For example, if solute transport is not simulated (**isol=0**), then solute related parameters do not need to be provided, because these will be part of *if(isol.ne.0)then..else..endif* statements. Note the following meanings of the logical operators: *.eq.* = equal to, *.ne.* = not equal to, *.gt.* = greater than, *.lt.* = lower than. The *do i=1,n* statement requires the instructions listed until *end do* to be repeated the stated number (*n*) times.

The user can put comments in the input file, provided these are on lines that start with an * (in the first column). Use spaces instead of commas to separate the various parameters on one line. Do not use tab stops in the input file. An example input file is given in Section II.1.3.

Input file structure:

input file for swim v2.1x

this line indicates that this is a SWIMv2.1 input file. It needs to be typed exactly as given; where x is a number between 0 and 9 or @. It indicates the version of SWIMv2.1 you are using. If x is the character @, then the output file is suitable for the program SWIMPLOT.

isol

solute flag (0 for no solute, 1 for solute)

t0,tfin,pint,dw

t0 = initial time (h)

tfin = final time (h)

pint = output time interval (h)

dw = water increment for the integration time step (cm)

dw determines the integration time step (see Section I.1.2). If the simulation suffers from instabilities, reduce this parameter value. Good results have been obtained using values of dw between 0.1 and 1.0. If a value lower than 0 is given for pint, then the print times will be read from the specified file (below) (one entry per line)

if(pint.lt.0)then

fname

file name for print times

endif

tcycle,ncult

tcycle = cycle time (h) (0 for no cycling)

ncult = number of cultivation times (max. MCT=20).

As explained in Section I.5.4, cultivation means that the surface may be disturbed or solute applied or both or neither. Alternatively or in addition, it provides SWIMv2.1 with points in time to solve to and, optionally, to print at (only to the screen/console) Surface disturbance resets the surface conductance and surface storage to their specified initial values (g1 and hm1; see Sections I.5.2 and I.5.3). With cycling, the specified times are repeated every cycle time (time=t0 is the start of the cycle). Note that SWIMv2.1 assumes there is no surface disturbance before the first cultivation time. In other words, if the first cultivation is not at time=t0 or if no cultivation times are given, the surface storage and surface conductance are at their minimum values (g0 and hm0, respectively)! If you want to start the simulation with the given initial values (g1 and hm1), then you need to specify a cultivation at time=t0.

if(ncult.gt.0)then

if(isol.ne.0)then

(tcult(i),iprnt(i),idist(i),slapp(i), i=1,ncult)

tcult(i) is the time of the cultivation (h)

iprnt(i) is a flag for printing output (1 for yes, 0 for no);

idist(i) is a flag for surface disturbance (1 for yes, 0 for no);

slapp(i) is amount of solute applied (per cm²)

Use a new line for each cultivation.

else

(tcult(i),iprnt(i),idist(i), i=1,ncult)

descriptions see above

end if

end if

dtmin,dtmax,ersoil,ernode,errex,dppl,dpnl,swt

dtmin = minimum integration time step size (h)

dtmax = maximum integration time step size (h)

ersoil = allowable flux balance error (in cm/h) for the soil profile as a whole

ernode = allowable flux balance error (in cm/h) at each node

errex = relative fraction of the plant water uptake rate at which the rate will become fixed

dppl = limit on increasing change in p during iterations (cm)

dpnl = limit on decreasing change in p during iterations (cm)

swt = space weighting for gravity flow (σ , Eq. (14), see Section I.1.2)

See Chapter I.6 for details. Recommended values: 0.000001 for ersoil and ernode, 0.01 for errex, 2 for dppl and 1 for dpnl. swt can have values from 0.5 to 1, corresponding to central to fully upstream spatial weighting (see Chapter I.6). When swt is between -1 and 0.5, SWIMv2.1 will use central space weighting until possible oscillation begins, at which point it gradually changes to upstream weighting. When swt is less than -1 the acceptable condition for central differencing is extended by a factor of -swt (see Chapter I.6).

if(isol.ne.0)then

slcerr,slswt

slcerr = convergence error for solute concentration

slswt = space weighting for convective solute flow (σ_s , Eq (60), see Section I.3.2)

See Chapter I.6 for details. Recommended value for slcerr is 0.000001. slswt can have values from 0.5 to 1, corresponding to central to fully upstream spatial weighting (see Chapter I.6). When slswt is between -1 and 0.5, SWIMv2.1 will use central space weighting until possible oscillation begins, at which point it gradually changes to upstream weighting. When slswt is less than -1 the acceptable condition for central differencing is extended by a factor of -slswt (see Chapter I.6). When experiencing negative concentrations and/or instabilities, try first to decrease the value of dw instead of moving the differencing upstream, as the latter causes increased numerical dispersion.

end if

psi0, psi1, hair, rad, groot

psi0 = hyperbolic sine transform parameter (ψ_0 , Eq. (6), see Section I.1.1)

psi1 = hyperbolic sine transform parameter (ψ_1 , Eq. (6), see Section I.1.1)

hair = relative humidity of air (h_a , see Section I.4.2)

rad = root radius (r_r , see Section I.4.3)

groot = root conductance (g_r , see Section I.4.3)

The hyperbolic sine transform parameters are discussed in Section I.1.1; suggested values are psi0 = -50 and psi1 = psi0/10. The relative humidity of air (hair) is suggested to be 0.5 (see Section I.4.2 on soil evaporation). The root radius (rad) and root conductance (groot) (see Section I.4.3) are user defined. SWIMv1 used 0.1 cm and $1.4 \cdot 10^{-7}$ cm² water/h/cm root, respectively.

nveg

number of vegetation types (maximum NV=4)

if(nveg.gt.0)then

do i=1,nveg

psimin(i),xc(i),rldmax(i),fevmax(i),vcycle(i),iroot(i),igrow(i)

psimin = minimum xylem potential (cm)

xc = root depth constant (cm)

rldmax = maximum root length density (cm/cm³)

fevmax = maximum fraction of potential evaporation

vcycle = vegetation cycle time (h) (0 for no cycling)

iroot = flag for cumulative root growth input (0 for exponential, 1 for depth - cumulative growth pairs, 2 for depth - time - growth values)

igrow = flag for growth input with time (0 for sigmoid, 1 linear interpolation)

For details see Section I.4.1 and I.4.3 and Example 1.2 in Section II.1.3.

if(iroot(i).eq.1)then

ndrt(i)

number of depth - root growth pairs (maximum MDRT=21).

(drt(j,i),grt(j,1,i), j=1,ndrt(i))

drt = depth

grt = cumulative root length fraction

Results in a table of ndrt(i) rows and two columns (drt and grt).

```

else if(iroot(i).eq.2)then
  ndrt(i),ntrt(i)
    ndrt = number of root growth depths (max. MDRT=21)
    ntrt = number of times (max. MTRT=25)

  (trt(j,i), j=1,ntrt(i))
    root growth times (line with ntrt(i) entries)

  (drt(j,i),(grt(j,k,i), k=1,ntrt(i)), j=1,ndrt(i))
    drt = depth
    grt = cumulative root length fraction for the different times
    Results in a matrix; see Example 1.2 and Table 3 in Section II.1.3.

end if

if(igrow(i).eq.0)then
  f1,t1,f2,t2,f3,t3,f4,t4
    fractions of maxima at corresponding times (see Example 1.2, Fig. 14-16)

else
  ntg
    number of time - growth pairs (max. MTG=25 in input file)
    If a value lower than 0 is given, the time - growth pairs will be read from the
    specified file (below).

  if(ntg.lt.0)then
    fname
      file name for time - growth pairs

  else
    (tg(1,j,i),tg(2,j,i), j=1,ntg)
      tg(1, .) = time
      tg(2,..) = growth
      Results in a table of ntg rows and two columns (tg(1,..) and tg(2,...)).

  end if

end if

end do

end if

ivap
  vapour flag (0, no vapour; 1, vapour conductivity is automatically added (see Section I.2.4))

nprop,slmin,slmax,hyscon
  nprop = number of soil hydraulic property points (maximum MP=1000)
  slmin = minimum value of log10 suction = xmin in HYPROPS input file (Section II.2.2)
  slmax = maximum value of log10 suction= xmax in HYPROPS input file (Section II.2.2)
  hyscon = ratio of scanning to dry-wet distances (>=1.5, 0 for no hysteresis)
  Except for the parameter hyscon this information comes from the output file of HYPROPS
  (see Sections I.2.1, I.2.2, and II.2). See Section I.2.6 for details relating to hyscon.

```

(sl(i),wc(i),wcd(i),hkl(i),hkld(i), i=1,nprop)

sl = \log_{10} suction

wc = water content

wcd = slope of water content vs. \log_{10} suction

hkl = \log_{10} conductivity

hkld = slope of \log_{10} conductivity vs. \log_{10} suction

This information (table of five columns and nprop rows) is copied from the output file of HYPROPS (see Sections II.2, I.2.1 and I.2.2, and Example 1.7 in Section II.1.3). It is, later in the input file, referred to as hydraulic property array.

if(isol.ne.0)then

slxc,slpmax,slpc1,slpc2,scycle,idepth,itime

slxc = solute production rate depth constant

slpmax = maximum production rate (per unit depth)

slpc1 = upper cutoff potential

slpc2 = lower cutoff potential

scycle = solute cycle time (0 for no cycling)

idepth = flag for solute production with depth (0 for exponential, 1 for depth - cumulative rate pairs, 2 for depth - time - cumulative rate values)

itime = flag for production rate input with time (0 for sigmoid, 1 for linear interpolation)

See Section I.3.4 and Example 1.3 in Section II.1.3.

if(slpmax.ne.0.)then

if(idepth.eq.1)then

ndsl

number of depth - solute production pairs (max. MDL=11).

(dsl(j),psl(j,1),j=1,ndsl)

dsl = depth

psl = cumulative production rate fraction

Results in a table of ndsl rows and two columns (dsl and psl).

else if(idepth.eq.2)then

ndsl,ntsl

ndsl = number of depths (max. MDL=11) for solute production

ntsl = number of times (max. MTS=11) for solute production

(tsl(j),j=1,ntsl)

solute production times (line with ntsl entries)

(dsl(j),(psl(j,k),k=1,ntsl),j=1,ndsl)

dsl = depth

psl = cumulative production rate fractions at given times

Results in a matrix; see Example 1.2 and Table 3 in Section II.1.3.

end if

if(itime.eq.0)then

f1,t1,f2,t2,f3,t3,f4,t4

fractions of maxima at corresponding times (see Example 1.3 in Section II.1.3)

else

ntspr

number of time - solute production rate pairs (max. MTSPR=25)

If a value lower than 0 is given, the time - solute production rate pairs will be read from the specified file (below).

if(ntspr.lt.0)then

fname

file name for time - solute production rate pairs.

else

(tspr(1,j,i),tspr(2,j,i), j=1,ntg)

tspr(1,) = time

tspr(2,...) = cumulative production rate fraction

Results in a table of ntg rows and two columns (tspr(1,...) and tspr(2,...)).

end if

end if

end if

slupf,slos,slsci,slscr,d0,a,dthc,dthp,disp

slupf = fraction of solute in plant water uptake that is actually taken up (Eq. 65)

slos = osmotic pressure per unit solute concentration (Eq. 88, Section I.4.4)

slsci = concentration in infiltration from solute applied to the surface (in cultivation)

slscr = concentration in runoff from solute applied to the surface (in cultivation)

d0 = ionic or molecular diffusion coefficient in free water (D_0 , Eq. (51))

a = tortuosity parameter (a , Eq. (52))

dthc = tortuosity parameter (b , Eq. (52))

dthp = tortuosity parameter (ξ , Eq. (52))

disp = hydrodynamic dispersion exponent (n , Eq. (51))

These solute-soil characteristics apply to all depths. Properties that are potentially depth dependent are specified below. See Section II.1.4 for an example of the calculation of slos. slsci and slscr give the concentrations at which the solute applied to the surface in a cultivation will dissolve in infiltration or runoff water. Solute concentration is expressed in terms of an amount of solute per cm^3 water (see Section I.3.1).

nprop

number of solute property points (max. MPSL=101).

(rhob,exco,fip(i),dis(i),alpha(i),beta, i=1,nprop)

rhob = bulk density (ρ , Eq. (50))

exco = Freundlich exchange isotherm coefficient (k , Eq. (53))

fip = Freundlich exchange isotherm exponent (η , Eq. (53))

dis = dispersivity (ε , Eq. (53))

alpha = liquid phase first order production rate coefficient ($-\lambda_1$, Eq. (64))

beta = solid phase first order production rate coefficient ($-\lambda_2$, Eq. (64))

Results in a table (6 columns and nprop rows). Later referred to as solute property array.

end if

initial water content

optional entry. Type the above sentence exactly to use initial water contents instead of initial matric potentials (specified below).

np

number of space grid points (depth nodes) (maximum M+1=251)

if(hyscon.eq.0d0)then

if(isol.eq.0)then

(x(i),psi(i),index(i,1), i=0,np-1)

else

(x(i),psi(i),index(i,1),csl(i),indxsl(i), i=0,np-1)

end if

else

if(isol.eq.0)then

(x(i),psi(i),index(i,1),dh,fh, i=0,np-1)

else

(x(i),psi(i),index(i,1),dh,fh,csl(i),indxsl(i), i=0,np-1)

end if

For each space grid point (depth node):

x = depth (see Fig. 2, Section I.1.2 and Fig. 11, Chapter I.6)

psi = initial matric potential (or initial water content if that option is used)

index = position in hydraulic property array; 0 interpolates between property sets of nodes above and below

dh = hysteresis value (<0, psi between curves; 0-1, no hysteresis; >1, multiple of psi relating curves); (see section I.2.6)

fh = fractional distance of psi between drying and wetting curves; 0 for drying, 1 for wetting; (see section I.2.6)

csl = solute concentration in soil water (amount per cm³)

indxsl = positions in solute property array

Choose for index(-) and indxsl(-) one (it does not matter which) position in the property array that represents the properties of the depth node (see Example 1.5 in Section II.1.3).

end if

if(isol.eq.0)then

h

h = initial height of surface water pond

else

h,cslsur

h = initial height of surface water pond

cslsur = initial solute concentration in surface water pond

end if

gf,isbc,itbc,ibp,ibbc

gf = gravity factor (cosine of angle between x direction and gravity); usually 1 (vertical flow), but can be different (e.g. 0 for horizontal flow). It is equal to $g = -dz/dx$ (Eq. 9)
isbc = surface boundary condition - 0 for no ponding (all runoff), 1 for ponding (no runoff), 2 for simple power-law runoff function (see Section I.5.3), 3 for simple power-law runoff function and specification of potential downslope flow within the soil (see Section I.1.3).
itbc = top boundary condition - 0 for infinite surface conductance, 1 for constant potential, 2 for conductance function (see section I.5.2)
ibp = bypass flow from runoff - 0 for no bypass flow, 1 for bypass flow (see Section I.2.5)
ibbc = bottom boundary condition - 0 for given matric potential gradient, 1 for given matric potential, 2 for zero flux, 3 for seepage above a certain threshold suction (see Section I.1.3)

if(isbc.eq.(2)

hm1,hm0,hrc,roff0,roff1

hm1 = initial surface storage ($h_{0initial}$, Eq. (98))
hm0 = minimum surface storage (h_{0min} , Eq. (98))
hrc = storage precipitation constant (Eq. (98))
roff0 = runoff factor (a , Eq. (99))
roff1 = runoff power (b , Eq. (99))

Parameters for surface roughness and simple power-law roff function (Section I.5.3).

end if

if(isbc.eq.3)

hm1,hm0,hrc,roff0,roff1,slope

Parameters in runoff function (as above)

slope = slope gradient (s , Eq. (15), for potential downslope flow, Section I.1.3)

end if

if(itbc.eq.2)

g1,g0,grc

g1 = initial surface conductance ($G_{initial}$, Eq. (95))
g0 = minimum surface conductance (G_{min} , Eq. (95))
grc = conductance precipitation constant (Eq. (95))
Parameters in surface conductance function (Section I.5.2).

end if

if(ibp.ne.0)then

xbp,gbp,sbp

xbp = depth for bypass flow
gbp = conductance for bypass flow (G_{bp} , Eq. (42))
sbp = storage (cm water per cm of positive ψ) for bypass flow
See Section I.2.5 for details.

end if

if(ibbc.eq.0.or.ibbc.eq.1.or.ibbc.eq.3)then

ntb

number of time - boundary condition pairs (max. MTB=500 in input file)

If a value lower than 0 is given, the time -boundary condition pairs will be read from the specified file

if(ntb.lt.0)then

fname

file name for time, boundary condition pairs.

else

(tb(1,i),tb(2,i), i=1,ntb)

tb(1,..) = time

tb(2,..) = boundary condition value

This value can be a matric potential gradient, matric potential or threshold suction for seepage depending on the boundary condition chosen.

end if

end if

if(isol.ne.0)then

if(ibbc.eq.1)

csl(n)

fixed solute concentration at bottom boundary if the bottom boundary condition is given as a matric potential (ibbc=1)

end if

nts

number of time - cumulative added amounts of solute pairs (in rainfall or irrigation)

See Example 1.7 in Section II.1.3) (max. MTS=500 in input file). If a value lower than 0 is given, the time - cumulative solute pairs will be read from the specified file (below).

if(nts.lt.0)then

fname

file name for time - cumulative solute pairs.

else

(ts(1,i),ts(2,i), i=1,nts)

ts(1,..) = time

ts(2,..) = cumulative solute (amount)

end if

end if

ntr

number of time - cumulative rain pairs (max. MTR=500 in input file). If a value lower than 0 is given, the time - cumulative rain pairs will be read from the specified file (below). First pair must be at time **t0** and have cumulative rain = 0.

if(ntr.ne.0)

effpar

effectiveness parameter (E_{ff} , see Section I.5.1)

end if

if(ntr.lt.0)then

fname

file name for time - cumulative rain pairs

else

(tr(1,i),tr(2,i), i=1,ntr)

tr(1,...) = time

tr(2,...) = cumulative rain (cm)

end if

ntr

number of time - cumulative potential evapotranspiration pairs (max. MTE=500 in input file). If a value lower than 0 is given, the time - cumulative evaporation pairs will be read from the specified file (below). First pair must be time **t0** and have value = 0.

if(ntr.lt.0)then

fname

file name for time - cumulative potential evapotranspiration pairs

else

(te(1,i),te(2,i), i=1,ntr)

te(1,...) = time

te(2,...) = cumulative potential evapotranspiration (cm)

end if

1.3 Examples

Example 1.1: Input file

An example input file for SWIMv2.1 is given in Table 1 below. In this example solute is applied through cultivation. This solute will enter the soil profile with the rainfall/irrigation. There is also some solute present initially. Solute production (see also Example 1.3) and first order decay processes are active. Two vegetation types are present with different growth patterns (see also Example 1.2). There is no solute exclusion from plant water uptake, i.e. all solute dissolved in the uptake water is also taken up by the plant. In this example vapour conductivity is not taken into account, nor is the effect of osmotic potential. There is one hydraulic property set and one solute property set, each applying to all 14 depth nodes of the 250 cm deep profile. The indexing of multiple property sets is illustrated in Example 1.5. Hysteresis is not taken into account, but Example 1.6 illustrates how this could be done. Runoff is governed by a simple power law function and a surface conductance function. The bottom boundary condition is "unit gradient". In the current example there is no solute input with rainfall or irrigation. Example 1.7 shows how this can be implemented. Table 2 shows an example of the output on the screen.

Table 1: Example input file for SWIMv2.1.

ex.in2	Comments
* example of swimev input file with solute	<i>Comment lines start with “*”</i>
* first line must be : input file for swim v2.11	<i>Version 2.11 is used; replace 1 by @ to see the output using SWIMPLOT</i>
* isol 1	<i>Solute is included in this simulation</i>
* t0,tfin,pint,dw 0 2400 24 1	<i>Start = 0 h, end = 2400 h, output every 24 h, water increment = 1 cm</i>
* tcycle,ncult 0 2	<i>No cycling, but 2 cultivations are carried out: at 0 h to disturb the surface and apply 1000 units of solute to the surface, and at 288 h to apply another 500 units of solute</i>
* ----- i=1,ncult -----	
* tcult(i),iprnt(i),idist(i),slapp(i) 0 0 1 1000 288 0 0 500	
* dtmin,dtmax,ersoil,ernode,errex,dppl,dpnl,swt 0 24 .000001 .000001 .01 2 1 0	<i>Recommended step sizes and limits, and central differencing until unstable</i>
* slcerr,slswt .000001 0	<i>Recommended solute error limit and central differencing until unstable</i>
* psi0,psi1,hair,rad,groot -50 -5 0.5 0.1 1.4d-7	<i>Recommended parameters for transform parameters, and relative air humidity, and SWIMv1 values for root radius and root conductance.</i>
* nveg 2	<i>2 vegetation types 1st crop: min. xylem potential= -15000 cm, exponential root growth with depth and sigmoid with time (root growth and potential evaporation) – see Example 1.2. 2nd crop: min.xylem potential= -25000 cm, exponential root growth with depth and sigmoid with time (root growth and potential evaporation) – see Example 1.2.</i>
* ----- i=1,nveg -----	
* psimin(i),xc(i),rldmax(i),fevmax(i),vcycle(i),	
* iroot(i), igrow(i)	
* f1,t1,f2,t2,f3,t3,f4,t4	
-15000 30 5 .5 0 0 0	
.2 0 .9 720 .2 0 .9 720	
-25000 100 1 .5 0 0 0	
.9 0 .95 720 .9 0 .95 720	
* ivap 0	
	<i>Vapour conductivity is not taken into account.</i>

Table 1 (continued): Example input file for SWIMv2.1.

ex1.in2 - continued	Comments
* nprop,slmin,slmax,hyscon 8 -3.000000 7.000000 0	<i>Output from HYPROPS (see Example 2.1 in Section II.2.3) is copied and a "0" for no hysteresis is added.</i>
* ---- i=1,nprop ---- * sl(i),wc(i),wcd(i),hkl(i),hkld(i) -3.000000 0.450000 -0.000000 0.518514 -0.000000 0.200000 0.449801 -0.000916 0.516249 -0.010432 0.800000 0.446849 -0.014511 0.482502 -0.166423 1.200000 0.430118 -0.091560 0.286939 -1.090903 1.400000 0.400243 -0.209453 -0.081968 -2.681818 3.175000 0.158094 -0.082733 -4.842196 -2.681818 5.475000 0.047445 -0.024829 -11.010377 -2.681818 7.000000 0.021360 -0.011178 -15.100151 -2.681818	<i>In this case there is only one hydraulic property set (containing 8 lines) that applies to all depth nodes (see below). The table is copied from the HYPROPS output (see Example 2.1 in Section II.2.3).</i>
* slxc,slpmax,slpc1,slpc2,scycle,idepth,itime 10 .1 -1000 -15000 0 0 0 * fl,t1,f2,t2,f3,t3,f4,t4 .1 240 .9 480 .9 480 .1 960	<i>Solute is produced in the profile following an exponential depth function and a sigmoid time function (see Example 1.3)</i>
* slupf,slos,slsci,slscr,d0,a,dthc,dthp,disp 1 0 5 2 0 0 0 1 1	<i>Solute is not excluded from plant water uptake (slupf=1), slos=0 to turn off the effect of the osmotic potential (see Example 1.4), surface applied solute enters infiltration and runoff water at concentrations of 5 and 2 units/cm³, respectively, d0=0 cm²/h (i.e. no diffusion), tortuosity=0, dispersion exponent disp = 1.</i>
* nprop 1 * ---- i=1,nprop ---- * rhob,exco,fip(i),dis(i),alpha(i),beta 1 3 1 2 -.01 -.005	<i>One solute property set applies to all depth nodes: bulk density=1 g/cm³, solute gets adsorbed (linear isotherm with exco=3 and fip=1), dispersion coefficient=2, first order decay coefficients are -0.1/h and -0.005/h, respectively.</i>
* np 14 * ---- i=1,np ---- * x(i),psi(i),index(i,1),csl(i),indxsl(i) 0 -300 1 5 1 1 -300 1 5 1 5 -300 1 5 1 10 -300 1 5 1 15 -300 1 5 1	<i>14 depth nodes are specified for each is given: depth, initial matric potential, index determining the hydraulic property set to be used (in this case the one and only one), initial solute concentration, and solute property set to be used</i>

Table 1 (continued): Example input file for SWIMv2.1.

ex1.in2 - continued	Comments
30 -300 1 5 1 45 -300 1 5 1 60 -300 1 0 1 75 -300 1 0 1 90 -300 1 0 1 120 -300 1 0 1 150 -1000 1 0 1 180 -1000 1 0 1 250 -1000 1 0 1	<i>(in this case the one and only one). See also Example 1.5.</i> <i>The profile is 250 cm deep with surface at 0 cm and bottom boundary condition applying at 250 cm.</i>
* h,cslsur 0 0	<i>Initially there is no water ponded on the surface and (hence) solute concentration of “ponded” water is zero.</i>
* gf,isbc,itbc,ibp,ibbc 1 2 2 1 0	<i>Vertical profile (gf=1), simple power law runoff function (isbc=2), conductance function (itbc=2), bypass flow turned on (ibp=1), given matrix potential gradient as bottom boundary condition</i>
* hm1,hm0,hrc,roff0,roff1 2 1 5 2 2	<i>Parameters for runoff function</i>
* g1,g0,grc 4 .02 2.5	<i>Parameters for conductance function</i>
* xbp,gbp,sbp 150 .1 .1	<i>Bypass flow from runoff goes 150 cm deep, the conductance = 0.1 /h and storage = 0.1 * matric potential at bypass node.</i>
* ntb 2 0 0 2400 0	<i>Two time-boundary condition pairs are specified, resulting in a matric potential gradient (ibbc=0) of 0 throughout the simulation, i.e. “unit gradient”</i>
* nts 0	<i>There is no solute input with rain or irrigation (see Example 1.5)</i>
* ntr 17	<i>17 time-cumulative rainfall records are specified below.</i>

Table 1 (continued): Example input file for SWIMv2.1.

ex1.in2 - continued	Comments
* effpar .184	<i>In the calculation of the amount of (2.5 cm/h) equivalent rainfall an effectiveness parameter of 0.184 is used.</i>
* ---- i=1,ntr ---- * tv(1,i),tv(2,i) 0 0 240 0 241 1 242 5 243 6 356 6 357 8 358 10 359 15 360 20 364 24 368 28 372 32 376 36 400 44 412 50 2400 50	<i>time-cumulative rainfall pairs: e.g. between 241 h and 242 h there was 4 cm of rain. Note that both rainfall and potential evapotranspiration can be specified in a file. In that case choose for ntr and nte negative numbers and specify the filenames instead of the time-rain/evaporation pairs. Example: for cumulative rain specified in the file ex1.rn: * ntr -1 * effpar .184 'ex1.rn' (include the '..')</i>
* nte 2 * ---- i=1,nte ---- * tv(1,i),tv(2,i) 0 0 2400 80	<i>Two time-cumulative potential evapotranspiration pairs are given. As the two times (0 and 2400 correspond to the start and final time of the run, this means that the 80 cm of potential evaporation was spread over the whole period (day and night!).</i>

Table 2: Example of screen output of the SWIMv2.1 run of ex1.in2.

day 30 hour 0 minute 0 second 0
water balance error = -.358E-04 cm water, with 5293. equations solved
evaporation rates for soil and vegetation in cm/h :
actual .002494 .015000 .015833
potential .002500 .015000 .015833
ET for soil and vegetation in cm :
actual 4.2157 7.0686 11.1396
potential 5.7918 7.0686 11.1396

Table 2 (continued): Example of screen output of the SWIMv2.1 run of ex1.in2.

```

water balance in cm :
rain runoff infil. drainage ET surface profile
50.0000 .0000 37.1299 16.3652 22.4239 .0000 61.8200
bypass flow in cm, cm/h :
depth store flow rate
150.00 .0000 12.8701 .0000
solute balance error = .160E-12, with 1404. equations solved
solute balance :
uptake by vegetation :
9.6282 8.4665
initially present: 847.1774
added - in rain or irrigation: .0000 - to surface: 1500.0000
- produced in profile: 299.5083
lost - in runoff: .0000 - in drainage: .0163
- by uptake: 18.0947 - by decay: 1177.2493
present - in surface water: .0000 - on surface: 1288.6103
- in profile: 162.7151
bypass flow :
depth store flow rate
150.00 .0000 25.7402 .0000
water variables in cm, cm/h :
depth potential water content conductivity flow rate
.00 -.163939E+04 .154842 .112559E-04 -.002494
1.00 -.146206E+04 .158926 .153009E-04 -.002202
5.00 -.114142E+04 .168097 .297211E-04 -.001670
15.00 -.810971E+03 .181585 .743281E-04 -.001852
30.00 -.538246E+03 .199181 .223143E-03 -.002732
45.00 -.388433E+03 .214420 .535181E-03 -.003325
60.00 -.303578E+03 .226732 .103652E-02 -.003394
75.00 -.251370E+03 .236653 .171938E-02 -.003019
90.00 -.216655E+03 .244783 .256136E-02 -.002262
120.00 -.174176E+03 .257251 .459887E-02 -.000142
150.00 -.149028E+03 .266559 .698664E-02 .002400
180.00 -.132500E+03 .273805 .957597E-02 .005346
250.00 -.118439E+03 .280908 .129373E-01 .012937
solute variables :
depth concn in water total concn dispersn coeff flow rate
.00 .492474E+01 .155368E+02 .322169E-01 .000000E+00
1.00 .366868E+01 .115891E+02 .277095E-01 -.434583E-02
5.00 .235983E+01 .747617E+01 .198748E-01 -.344335E-02
15.00 .100545E+01 .319892E+01 .203929E-01 -.130954E-02
30.00 .359995E+00 .115169E+01 .274328E-01 -.729043E-03
45.00 .178961E+00 .575256E+00 .310159E-01 -.412342E-03
60.00 .610448E-01 .196975E+00 .299397E-01 -.139740E-03
75.00 .145500E-01 .470934E-01 .255149E-01 -.289109E-04
90.00 .194267E-02 .630355E-02 .184798E-01 -.421252E-05
120.00 .638060E-03 .207832E-02 .110610E-02 -.312199E-07
150.00 .311742E-01 .101832E+00 .180082E-01 .627994E-04
180.00 .468354E-02 .153330E-01 .390488E-01 .100792E-03
250.00 .551534E-03 .180953E-02 .921105E-01 .754637E-05

```

Example 1.2: Root distribution

In the input file *ex1.in2* of Example 1.1, the flag **igrow(i)=0** means that the time functions for potential evaporation and root distribution are identical and are sigmoidal. As explained in Section I.4.1 a sequence of two functions can be described by defining two points on each curve: (f1,t1) and (f2,t2) on the first curve and (f3,t3) and (f4,t4) on the second curve. If the two pairs of points are identical as in Example 1.1, then only one function is used. The functions for the two vegetation types of Example 1.1 are shown in Fig. 14. If two different functions are specified (Fig. 15), SWIMv2.1 determines the intersection point of these two functions and defines the sequence as shown.

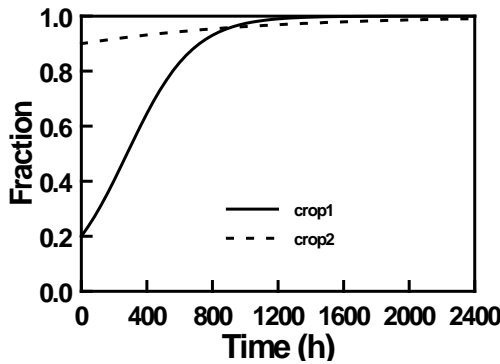


Figure 14: Sigmoid time functions for the two vegetation types of Example 1.1.
crop 1: f1=0.2, t1=0, f2=0.9, t2=720;
crop 2: f1=0.9, t1=0, f2=0.95, t2=720.

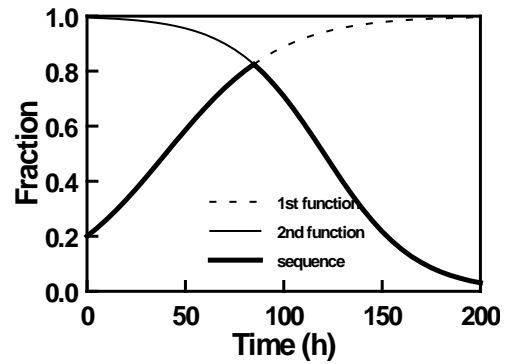


Figure 15: Sequence of two sigmoid time functions. function 1: f1=0.2, t1=0, f2=0.8, t2=80; function 2: f1=0.9, t1=70, f2=0.3, t2=140.

When a cycle time (**vcycle(i)**) is specified, SWIMv2.1 determines both the first and second intersection points. Depending on the relative positions of the cycle time and the intersections, sudden changes in fraction can occur (see Fig. 16).

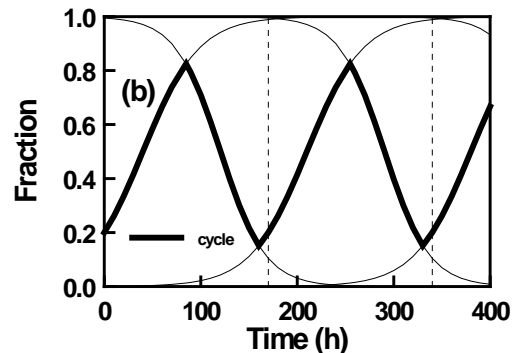
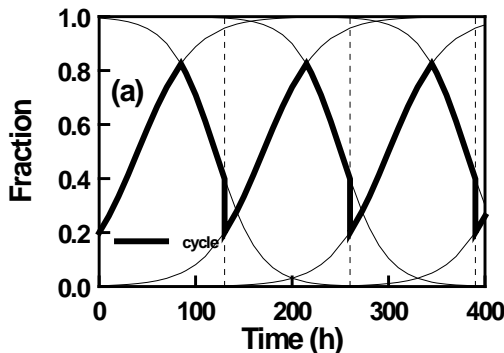


Figure 16: Definition of cycling for the case where (a) the cycle is before the second intersection, and (b) where it is after the second intersection. In (a) $vcycle=130$, in (b) $vcycle=160$. f1=0.2, t1=0, f2=0.8, t2=80, f3=0.9, t3=70, f4=0.3, t4=140.

The exponential depth function for the root distribution of Example 1.1 (due to **iroot(i)=0**) is given in Fig. 17. The root depth constant (**xc(i)**) is the depth at which the root length density fall to 37% of that at the surface.

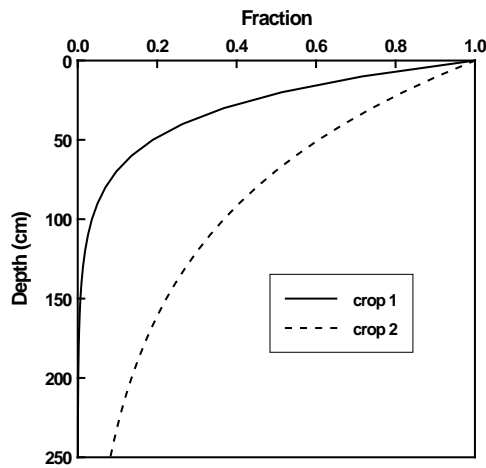


Figure 17: Exponential depth function for the root distribution of the two crops of Example 1.1. The root depth constant (**xc(i)**) was 30 cm for crop 1 and 100 cm for crop 2.

To calculate the root length density profiles at a given time, SWIMv2.1 multiplies the maximum root length density (**rldmax(i)**) with the fraction of the sigmoid time function and the exponential depth function fractions. The resulting root length density profiles for three different times are given in Fig. 18.

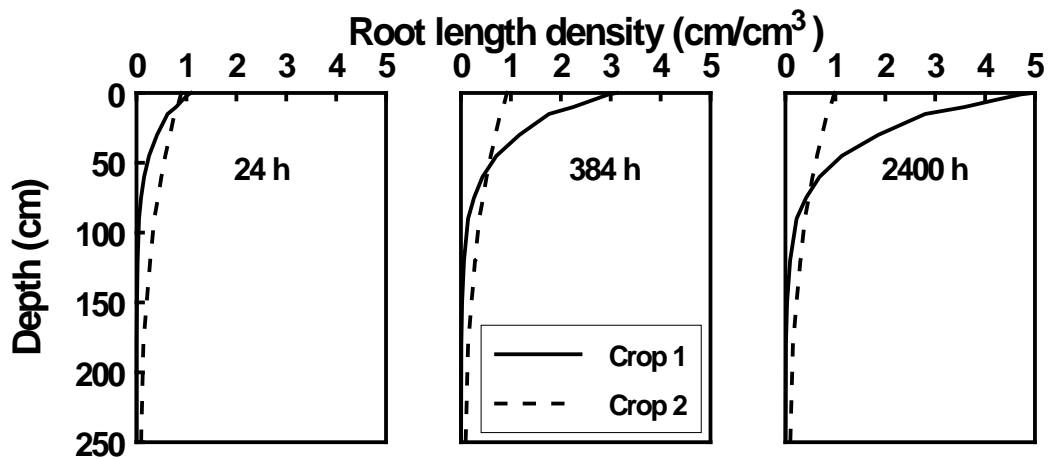


Figure 18: Root length density profiles at three different times (24, 384 and 2400 h) during the SWIMv2.1 run of the file *ex1.in2* of Example 1.1.

If instead of **iroot(i)=0**, one chooses **iroot(i)=2**, the root distribution profile is defined by a matrix of relative root length density with depth and time (see Section I.4.1). The depth component of this matrix is given as cumulative values with depth. The creation of such a matrix is illustrated below in Table 3. The first step is to write down the depth nodes defined elsewhere in the SWIMv2.1 input file (first column). For each node, determine the corresponding layer, using Fig. 2 in Section I.1.2 (column 2). The layer boundaries are exactly half-way between the nodes, except when a layer interface is forced to be at a node by defining two depth nodes with the same depth (see Section I.6). For each layer decide on the required the root length densities for the chosen times (column 3 and 4). In the example below two profiles are defined. By using the first (column 3) for both 0 h and 600 h (see Table 4), a constant root length density profile is obtained between 0 and 600 h, followed by a gradual change to the second profile (column 4) at 1200 h. Determine the maximum root length density at any time (**rldmax(i)**) and divide by this number to obtain the fractions of maximum root length density in columns 5 and 6. In column 7 the depths of the layer interfaces are recorded. To obtain the required cumulative values with depth the fractions of maximum root length density (columns 5 and 6) are integrated with depth (using column 7) to obtain columns 8 and 9 (for input to SWIMv2.1). The integration starts at the surface (0 cm) and moves down the column, multiplying the fraction of maximum root length density of a layer with the thickness of this layer and adding this number to the number in the previous row. The cumulative records are used in the input file (Table 4).

Table 3: Example calculations for the specification of root distribution with time and depth (option **iroot(i)=2).**

node	layer	user preparation					user input	
		rld wanted (0-600 h)	rld wanted (1200 h)	fr. max rld (0-600 h)	fr. max rld (1200 h)	layer interfaces	cum. fr. (0-600 h)	cum. fr. (1200 h)
0	0-0.5	5	5	1	1	0	0	0
1	0.5-3	4.75	4.75	0.95	0.95	0.5	0.5	0.5
5	3-7.5	4.375	4.375	0.875	0.875	3	2.875	2.875
10	7.5-15	3.75	3.75	0.75	0.75	7.5	6.8125	6.8125
20	15-25	3	3	0.6	0.6	15	12.4375	12.4375
30	25-35	2	2.25	0.4	0.45	25	18.4375	18.4375
40	35-45	1.25	2	0.25	0.4	35	22.4375	22.9375
50	45-55	0.5	1.75	0.1	0.35	45	24.9375	26.9375
60	55-65	0	1.5	0	0.3	55	25.9375	30.4375
70	65-75	0	1.25	0	0.25	65	25.9375	33.4375
80	75-85	0	1	0	0.2	75	25.9375	35.9375
90	85-95	0	0.75	0	0.15	85	25.9375	37.9375
100	95-105	0	0.5	0	0.1	95	25.9375	39.4375
110	105-115	0	0	0	0	105	25.9375	40.4375
120	115-125	0	0	0	0	115	25.9375	40.4375
130	125-135	0	0	0	0	125	25.9375	40.4375
140	135-145	0	0	0	0	135	25.9375	40.4375
150	145-155	0	0	0	0	145	25.9375	40.4375
160	155-165	0	0	0	0	155	25.9375	40.4375
170	165-170	0	0	0	0	165	25.9375	40.4375
						170	25.9375	40.4375

Table 4: Structure for root section of input file based on calculations in Table 3.

Input file structure								Comments
-15000	80	5	.8	0	2	0		<i>parameters and flags; xc=80 is not used</i>
21	3							<i>21 depth entries and 3 time entries</i>
	0			600		1200		<i>3 times</i>
0	0			0		0		<i>depth and entries for the 3 times</i>
0.5	0.5			0.5		0.5		
3	2.875			2.875		2.875		
7.5	6.8125			6.8125		6.8125		
15	12.4375			12.4375		12.4375		
25	18.4375			18.4375		18.4375		
35	22.4375			22.4375		22.9375		
45	24.9375			24.9375		26.9375		
55	25.9375			25.9375		30.4375		
65	25.9375			25.9375		33.4375		
75	25.9375			25.9375		35.9375		
85	25.9375			25.9375		37.9375		
95	25.9375			25.9375		39.4375		
105	25.9375			25.9375		40.4375		
115	25.9375			25.9375		40.4375		
125	25.9375			25.9375		40.4375		
135	25.9375			25.9375		40.4375		
145	25.9375			25.9375		40.4375		
155	25.9375			25.9375		40.4375		
165	25.9375			25.9375		40.4375		
170	25.9375			25.9375		40.4375		
.8	0	.95	370	.95	500	.85	706	<i>parameters for sigmoid time function for fraction of potential evaporation</i>

Example 1.3: Solute production

Solute production in Example 1.1 was given as a sequence of two functions. As with the definition of the time function for root distribution, SWIMv2.1 determines the intersection between the two curves and defines the overall time function as shown in Fig. 19.

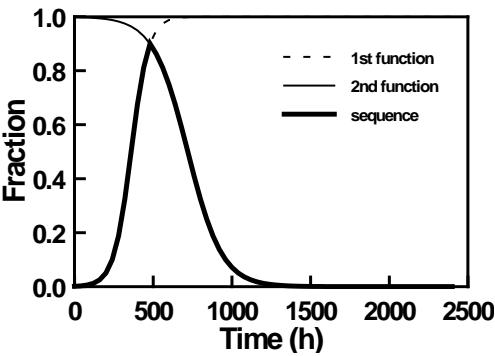


Figure 19: Time function for solute production used in Example 1.1. function 1: f1=0.1, t1=240, f2=0.9, t2=480; function 2: f1=0.9, t1=480, f2=0.1, t2=960.

Example 1.4: Calculation of **slos**

In Example 1.1, the effect of the osmotic potential on soil evaporation and root water uptake was eliminated by setting **slos** to zero. The value of **slos** depends not only on the type of solute and absolute temperature, but also on the units of solute concentration (Section I.4.3). Here we will present an example of the calculation of the value of **slos**.

The equation for the osmotic potential (Eq. 88) is based on the solute concentration unit of [$\mu\text{mol}/\text{cm}^3$]. If the solute concentration unit is different, the right-hand side of Eq. (88) must be multiplied by a conversion factor. Suppose we have a solute, its concentration is dilute enough to assume $\chi=1$, and the absolute temperature is 293K. Then **slos** is given by

$$\begin{aligned}\mathbf{slos} &= \nu \chi RT / (g \rho_w) \\ &= \nu \times 1 \times 8.3143 \times 10^{-2} \times 293 / (9.81 \times 10^2 \times 1.0 \times 10^{-3}) \\ &= \nu \times 24.83 [\text{cm cm}^3 / \mu\text{mol}]\end{aligned}$$

where the gravitational constant g is assumed to be equal to $9.81 \times 10^{-2} \text{ cm/s}^2$ and the density of water ρ_w $1.0 \times 10^{-3} \text{ kg/cm}^3$. For a solute that dissociates into 2 particles ($\nu=2$) and has a concentration of $100 [\mu\text{mol}/\text{cm}^3]$ this results in an osmotic potential ψ_o of -4970 cm. This value corresponds well with the plot of osmotic potential vs. concentration for NaCl in McIntyre (1980).

Note that the concentration c in Eq. (88) is the total molar concentration of the solution. For a solution containing a single solute, such as calcium chloride (CaCl_2), with a concentration of $10 \mu\text{mol}/\text{cm}^3$ (=mmol/L), $\nu=3$, **slos** = $3 \times 24.83 = 74.5$, and $\psi_o = -745 \text{ cm}$. However, if SWIMv2.1 is used to simulate chloride movement, and the concentration of chloride was $10 \mu\text{mol}/\text{cm}^3$ (=mmol/L), then the total molar concentration of CaCl_2 is $5 \mu\text{mol}/\text{cm}^3$ (=mmol/L) and (with $\nu=3$, and **slos** = $3 \times 24.83 = 74.5$) $\psi_o = -372.5 \text{ cm}$.

If, as is common place, the concentration being used is in mg/L or, in SWIMv2.1 units, $\mu\text{g}/\text{cm}^3$, then **slos** is given by

$$\mathbf{slos} = \nu \times 24.83 / M [\text{cm cm}^3 / \mu\text{g}]$$

where

M = molecular weight of the undissociated solute [g/mol = $\mu\text{g}/\mu\text{mol}$]

For the example of calcium chloride above, $M = 111$, so that **slos** = 0.67. For sodium chloride, $\nu = 2$, $M = 58.5$, and **slos** = 0.85.

If SWIMv2.1 is used to simulate the movement of total salt, this will usually be expressed in mg/L or, in SWIMv2.1 units, $\mu\text{g}/\text{cm}^3$ and represent all species present. In that case,

$$\mathbf{slos} = 24.83 / \bar{M} [\text{cm cm}^3 / \mu\text{g}]$$

where

\bar{M} = weighted average ionic ($\nu = 1!$) weight of all species present [g/mol = $\mu\text{g}/\mu\text{mol}$]

The average ionic weight of ions commonly found in soil water (MgCl_2 , CaCl_2 , NaCl , MgSO_4 , Na_2SO_4 , and NaHCO_3) is 41. Using this value, **slos** becomes 0.61.

Example 1.5: Hydraulic properties

In the input file *ex1.in2* of Example 1.1 only one hydraulic property set was defined and hence the array position (**index(i,1)**) for each depth node was equal to 1. Table 5 below illustrates how multiple hydraulic property sets can be defined and how these are assigned to the different depth nodes. Three property sets were generated using HYPROPS (Section II.2) and combined into one table (column 3). In this case each set consisted of 11 lines, so that the total number of lines is 33. Set 1 starts on line 1, set 2 on line 12 and set 3 on line 23. To each depth node (column 4) a property set is assigned by setting the parameter **index(i,1)** equal to the first line number of that set. For example, the depth node at 90 cm uses hydraulic property set 2 (which starts at line 12), and the node at 120 cm uses set 3 (which starts at line 23). If **index(i,1)** is set equal to zero (e.g. the node at 15 cm) SWIMv2.1 interpolates between the property sets above and below. We, therefore, have a gradual transition from layer 1 (nodes 0,1,5,10) to layer 2 (nodes 15,30,45,60, 75, 90). A sharper transition (layer 2 to 3) is at 105cm (between the nodes at 90 cm and 120 cm).

Table 5: Defining multiple hydraulic property sets

Line	Set	Hydraulic property table in input file					Depth nodes in input file
		33	-3.000000	7.000000	0		* np
1	1	-3.000000	0.377000	-0.000000	0.638489	-0.000000	14
2		-2.300000	0.377000	-0.000000	0.638489	-0.000001	* ---- i=1,np ----
3		-1.600000	0.377000	-0.000002	0.638484	-0.000023	* x(i),psi(i),index(i,1),
4		-0.900000	0.376991	-0.000042	0.638362	-0.000587	*no solute present
5		-0.200000	0.376772	-0.001051	0.635285	-0.014758	0 -300 1
6		0.400000	0.373382	-0.016662	0.587483	-0.236027	1 -300 0
7		0.763118	0.357737	-0.088710	0.361091	-1.311559	5 -300 0
8		0.925532	0.336491	-0.168829	0.037261	-2.653700	10 -300 1
9		2.836684	0.128983	-0.064715	-5.034362	-2.653700	15 -300 0
10		5.370627	0.036173	-0.018149	-11.758687	-2.653700	30 -300 12
11		7.000000	0.015972	-0.008013	-16.082554	-2.653700	45 -300 0
12	2	-3.000000	0.377000	-0.000000	0.459392	-0.000000	60 -300 0
13		-2.300000	0.377000	-0.000000	0.459392	-0.000001	75 -300 0
14		-1.600000	0.377000	-0.000002	0.459387	-0.000023	90 -300 12
15		-0.900000	0.376991	-0.000042	0.459265	-0.000587	120 -300 23
16		-0.200000	0.376772	-0.001051	0.456189	-0.014758	150 -1000 0
17		0.400000	0.373382	-0.016662	0.408387	-0.236027	180 -1000 0
18		0.763118	0.357737	-0.088710	0.181994	-1.311559	250 -1000 23
19		0.925532	0.336491	-0.168829	-0.141836	-2.653700	
20		2.836684	0.128983	-0.064715	-5.213459	-2.653700	
21		5.370627	0.036173	-0.018149	-11.937784	-2.653700	
22		7.000000	0.015972	-0.008013	-16.261651	-2.653700	
23	3	-3.000000	0.297000	-0.000000	0.309630	-0.000000	
24		-2.300000	0.297000	-0.000000	0.309630	-0.000001	
25		-1.600000	0.297000	-0.000001	0.309625	-0.000023	
26		-0.900000	0.296993	-0.000033	0.309503	-0.000587	
27		-0.200000	0.296820	-0.000828	0.306426	-0.014758	
28		0.400000	0.294150	-0.013127	0.258624	-0.236027	
29		0.763118	0.281825	-0.069886	0.032232	-1.311559	
30		0.925532	0.265087	-0.133003	-0.291598	-2.653700	
31		3.004730	0.093397	-0.046860	-5.809166	-2.653700	
32		5.807288	0.022890	-0.011485	-13.246314	-2.653700	
33		7.000000	0.012582	-0.006313	-16.411413	-2.653700	

Example 1.6: Specification of hysteresis parameters

If hysteresis is to be included in the SWIMv2.1 simulation runs, the parameters **dh**, **fh**, and **hyscon** need to be specified (Section I.2.6). To determine the value of the various hysteresis parameters, follow the steps outline below. It is assumed that measured or estimated hysteresis curves are available.

1. Describe the measured drying curve with one of the water retention functions given in Section I.2.1.
2. Check whether the wetting curve is best described by shifting the function of the drying curve on a liner scale (Eq. (44)) or log scale (Eq. (45)). In either case, determine the shift (= **dh**). **dh** will be negative if the shift is on a linear scale, or positive and larger than 1 in the case of a shift on log-log scale. **dh** needs to be specified for each depth node, but would usually only differ for the different hydraulic property sets.
3. For each measured scanning curve, calculate the difference between ψ_0 (point where it meets the main drying curve) and ψ_1 (point where it meets the wetting curve). Divide this difference by the shift **dh** to obtain **hyscon** (see also Eq. (46)). Note that if the shift **dh** was on a log scale, this calculation must be done on a log scale as well. **hyscon** needs to be at least 1.5. It is likely that the various experimental scanning curves result in different values for hyscon. SWIMv2.1 allows, however, only one value for hyscon for the whole profile. It will be necessary to pick the value that best describes the complete set of scanning curves.
4. The third parameter that is required is **fh**. It needs to be specified for each depth node (to accompany the specified initial matric potential or water content). It determines whether the initial matric potential or water content is on the drying curve (**fh**=0), on the wetting curve (**fh**=1), or on a scanning curve (**fh** between 0 and 1). **fh** is the initial value of z in Eq. (47).

Example 1.7: Solute input with rainfall/irrigation

If solute is added to the system with the rainfall or irrigation, a cumulative record of total solute with time needs to be specified (**nts**, **ts(1,i)**, **ts(2,i)**) (see Section II.1.2). This record is obtained by multiplying the known solute concentration in the rainfall or irrigation water with the amount of rainfall or irrigation. See also Section I.3.3. For example, if water is added at a rate of 0.36 cm/h for 13.5 h and this water contains 200 mmol/L bromide, then the 4.86 cm of water added contained 972 μmol of bromide. The input file structure then looks like:

```

2
0      0
13.5   972
2
0.184
0      0
13.5   4.86

```

2. USING HYPROPS TO GENERATE HYDRAULIC PROPERTY INPUT

Before running the SWIMv2.1 model (see Section II.1), it is necessary to convert measured or estimated hydraulic properties into a form that the SWIMv2.1 program accepts. For this purpose the program HYPROPS is provided. This program needs to be run first, as its output is used to prepare the SWIMv2.1 input file (see Example 2.1 in Section II.2.3). HYPROPS is not a hydraulic property fitting program. The user needs to provide the parameter values of the functions that are chosen to describe the water retention and conductivity data. HYPROPS performs any necessary summations according to Eq. (31) and (32), and generates a hydraulic property table based on a piecewise cubic approximation. See Sections I.2.1 and I.2.2 for details.

2.1 Running HYPROPS

To run HYPROPS type the following line at the DOS prompt:

hyprops

The program first requests the user to enter the input file *filename.spg*. After that HYPROPS presents the user with five options:

- 0 cubic approximation. An output file (*filename.sps*) needs to be given when requested for, as this output file is needed to run SWIMv2.1. The conversion of this output file to SWIMv2.1 input is shown in Example 2.1 in Section II.2.3.
- 1 plot θ vs. $\log(-\psi)$, with the option to print the data to a file (*filename.thh*)
- 2 plot $-d(\theta)/d(\log(-\psi))$ vs. $\log(-\psi)$, with the option to print the data to a file (*filename.ch*)
- 3 plot $K(\psi)$ vs. $\log(-\psi)$, with the option to print the data to a file (*filename.kh*)
- 4 plot $K(\theta)$ vs. θ , with the option to print the data to a file (*filename.kth*)

Choose an option by typing its number. Any other number will exit the program. Option 2 reflects the pore size distribution $f(\psi)$ (see Section I.2.1).

2.2 Preparing the input file for HYPROPS

The input file structure for HYPROPS is given below. The **bold** parameters need to be provided by the user, as specified by the instructions. Comments can only be placed at the end of the input file. Separate the various parameters on one line by commas.

xmin, xmax

xmin and xmax set the range of $x = \log_{10} \psi$, usually xmin = -3 and xmax = 7.

nsets

nsets is the number of data sets - one for each soil layer with distinct hydraulic properties. HYPROPS does not specify a maximum number of nsets, but SWIMv2.1 has a limit of 1000 lines of HYPROPS output (see Sections II.1.2 and II.2.3).

for each set

colour,thr,ths

colour for plots, residual (θ_r) and saturation water contents (θ_s)
(for colour there are the following choices: r=red, o=orange, y=yellow, g= green,
b=blue, i=indigo, v=violet, B=black, W,w=white, G=grey)

nc

number of components (maximum 5) = non-interacting pore-spaces (see Section I.2.2)

for each component

cfrac,hks,fun,p1,p2,p3

fractional contribution of this component, saturated hydraulic conductivity (for components in parallel), model for hydraulic conductivity function, and parameters for that model:

fun = mu - Mualem's model (Eq. 25)

p1=pore interaction index p

p2=0

p3=0

fun=bc - Brooks-Corey function (Eq. 27)

p1=pore interaction index p

p2= $\lambda=1/b$

p3=0

fun = vg - Van Genuchten function (Eq. 28)

p1=pore interaction index p

p2= n

p3= m

nterms

number of terms in this component (maximum 5)

for each term

tfrac,fun,p1,p2,p3

fractional contribution of this term, water retention curve model and its parameters:

fun = uc - unsmoothed Brooks-Corey function (Eq. 18)

fun = bc - smoothed Brooks-Corey function (Eq. 19)

p1= $\alpha = -1/\psi_e = -1/\text{air entry potential}$

p2= $\lambda=1/b$

p3=0

fun = um = modified, unsmoothed Brooks-Corey function (Eq. 20)

fun = mc = modified, smoothed Brooks-Corey function (Eq. 21)

p1= $\alpha = -1/\psi_e = -1/\text{air entry potential}$

p2= $\lambda=1/b$

p3= $\alpha_{haz} = -1/\psi_0 = -1/\text{oven dry potential} = 10^{-7} \text{ cm}^{-1}$

fun = vg - van Genuchten function (Eq. 22)

p1= α

p2= n

p3= m , if p3=0 then $m=1-1/n$ is assumed

fun = ex - one parameter exponential function (Eq. 23)

p1= $\alpha = a_{ex} = \text{constant}$

p2=0

p3=0

next term

next component

next set

2.3 Examples

Example 2.1

An example input file for HYPROPS is given in Table 6. The file provides the parameterisation of two soil types that are both described by **bc** type (see Sections I.2.1 and I.2.2) hydraulic properties. The resulting output file is given in Table 7. The output consists of blocks of data corresponding to the property sets defined in the input file. Each set starts with a line specifying the number of lines in the following block and the **xmin** and **xmax** values given. In Table 7, there are two property sets with 12 and 8 lines, respectively. The five columns of the blocks of data represent the $\log_{10}|\psi|$, water content θ , the slope of θ vs. $\log_{10}|\psi|$, $\log_{10} K$, and the slope of $\log_{10} K$ vs. $\log_{10}|\psi|$.

The HYPROPS output file needs to be modified only slightly before it can be inserted into the SWIMv2.1 input file. Instead of having a line with the number of lines and **xmin** and **xmax** for each property set, SWIMv2.1 only needs one such line at the top, specifying the total number of lines (Table 8).

The plots of the water content (θ), pore size distribution ($f(\psi)$), and hydraulic conductivity (K) versus soil suction ($-\psi$) are presented in Fig. 20. Comparison of Figs. 20a and 20b shows nicely the link between pore size distribution and the water retention curve.

Table 6: HYPROPS input file for Example 2.1

Input file	Comments
-3,7	<i>min and max values for $\log_{10}(-\psi)$</i>
2	<i>2 data sets</i>
r,0.0,0.3	<i>red colour for 1st data set, $\theta_r=0.0$ and $\theta_s=0.3$</i>
1	<i>data set has 1 component</i>
	<i>contribution of this component to overall water retention curve of data set</i>
1,0.1,bc,1,0.25,0	<i>is 1, $K_s=0.1$, bc hydraulic conductivity function, $p=1$, $b=4$</i>
1	<i>component has one term</i>
	<i>contribution of this term to water retention curve of this component is 1,</i>
1,bc,0.05,0.25,0	<i>bc water retention curve, $\psi_e=-20$, $b=4$</i>
g,0.0,0.48	<i>green colour for 2nd data set, $\theta_r=0.0$ and $\theta_s=0.48$</i>
1	<i>data set has 1 component</i>
	<i>contribution of this component to overall water retention curve of data set</i>
1,0.1,bc,1,0.04,0	<i>is 1, $K_s=0.1$, bc hydraulic conductivity function, $p=1$, $b=25$</i>
1	<i>component has one term</i>
1,bc,1,0.04,0	<i>contribution of this term to water retention curve of this component is 1,</i>
	<i>bc water retention curve, $\psi_e=-1$, $b=25$</i>

Table 7: HYPROPS output

12	-3.000000	7.000000			
	-3.000000	0.300000	-0.000000	-1.000000	-0.000000
	-2.300000	0.300000	-0.000000	-1.000000	-0.000000
	-1.600000	0.300000	-0.000000	-1.000000	-0.000002
	-0.900000	0.299999	-0.000002	-1.000008	-0.000038
	-0.200000	0.299987	-0.000060	-1.000206	-0.000948
	0.500000	0.299675	-0.001496	-1.005175	-0.023844
	1.100000	0.294852	-0.023705	-1.082681	-0.384075
	1.442523	0.275074	-0.114786	-1.414381	-1.993503
	1.621602	0.249447	-0.143593	-1.881572	-2.750000
	3.459617	0.086591	-0.049846	-6.936114	-2.750000
	5.970298	0.020408	-0.011748	-13.840488	-2.750000
	7.000000	0.011282	-0.006494	-16.672168	-2.750000
8	-3.000000	7.000000			
	-3.000000	0.480000	-0.000000	-1.000000	-0.000001
	-2.300000	0.480000	-0.000000	-1.000004	-0.000019
	-1.600000	0.479998	-0.000010	-1.000106	-0.000487
	-0.900000	0.479945	-0.000255	-1.002658	-0.012240
	-0.200000	0.478608	-0.006411	-1.066852	-0.308311
	0.172964	0.472245	-0.035714	-1.374923	-1.740724
	0.359499	0.464367	-0.042770	-1.762138	-2.120000
	7.000000	0.251908	-0.023202	-15.840000	-2.120000

Table 8: input to SWIMv2.1

20	-3.000000	7.000000	0		
	-3.000000	0.300000	-0.000000	-1.000000	-0.000000
	-2.300000	0.300000	-0.000000	-1.000000	-0.000000
	-1.600000	0.300000	-0.000000	-1.000000	-0.000002
	-0.900000	0.299999	-0.000002	-1.000008	-0.000038
	-0.200000	0.299987	-0.000060	-1.000206	-0.000948
	0.500000	0.299675	-0.001496	-1.005175	-0.023844
	1.100000	0.294852	-0.023705	-1.082681	-0.384075
	1.442523	0.275074	-0.114786	-1.414381	-1.993503
	1.621602	0.249447	-0.143593	-1.881572	-2.750000
	3.459617	0.086591	-0.049846	-6.936114	-2.750000
	5.970298	0.020408	-0.011748	-13.840488	-2.750000
	7.000000	0.011282	-0.006494	-16.672168	-2.750000
	-3.000000	0.480000	-0.000000	-1.000000	-0.000001
	-2.300000	0.480000	-0.000000	-1.000004	-0.000019
	-1.600000	0.479998	-0.000010	-1.000106	-0.000487
	-0.900000	0.479945	-0.000255	-1.002658	-0.012240
	-0.200000	0.478608	-0.006411	-1.066852	-0.308311
	0.172964	0.472245	-0.035714	-1.374923	-1.740724
	0.359499	0.464367	-0.042770	-1.762138	-2.120000
	7.000000	0.251908	-0.023202	-15.840000	-2.120000

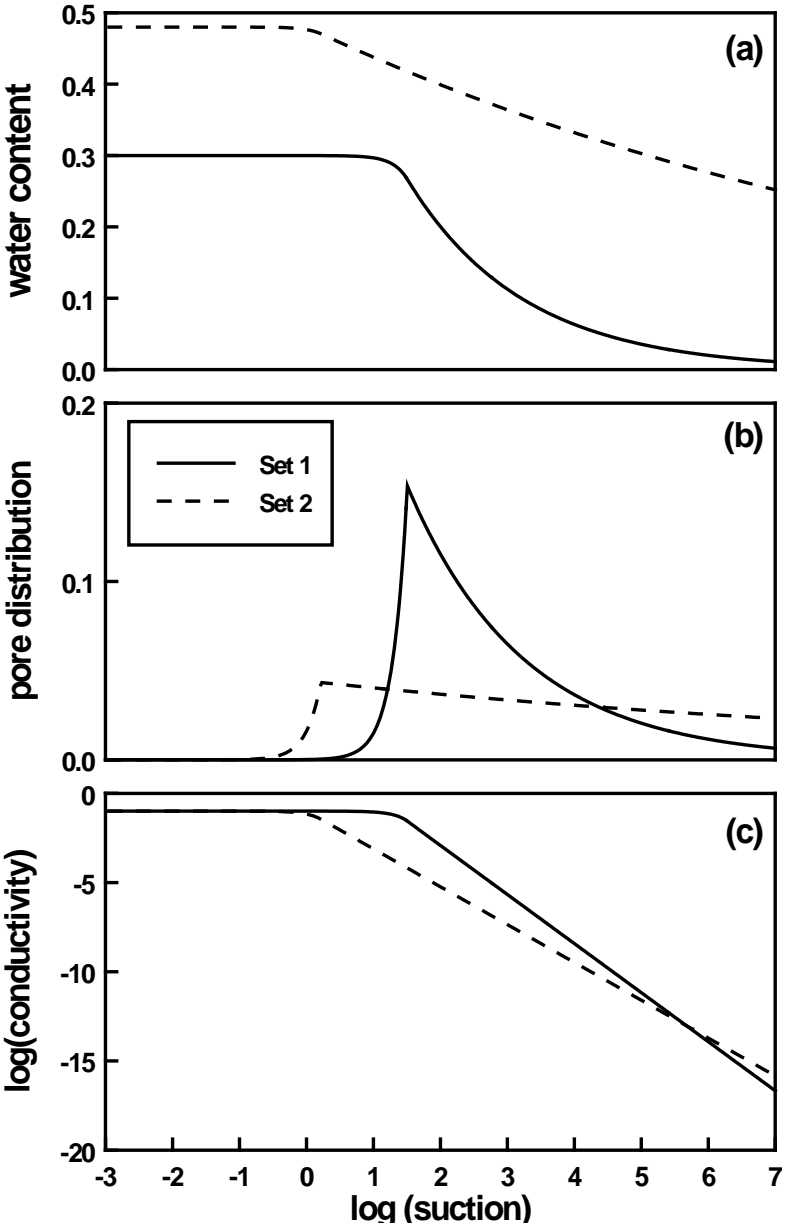


Figure 20: (a) water retention curves, (b) pore-size distributions, and (c) hydraulic conductivity functions for the two soil types (Set 1 and 2, see Table 6) of Example 2.1. The pore size distribution is represented by $-d\theta/d(\log_{10}-\psi)$. Suction is given by $(-\psi)$.

Example 2.2

Figure 21 illustrates the differences between the **uc** and **bc** descriptions of the water retention curve (a,b) and between the **bc** and **mu** descriptions of the hydraulic conductivity function (c). The **bc** water retention curve is smoother near the air-entry value than the **uc** water retention curve. The choice of **bc** or **mu** for hydraulic conductivity (Table 9) does not affect the description of the water retention curve. The hydraulic conductivity function described by a **bc** hydraulic conductivity curve with a **bc** water retention curve is intermediate to the two **mu** hydraulic conductivity functions with **uc** and **bc** water retention curves, respectively. A **bc** hydraulic conductivity function in combination with a **uc** water retention curve is the same as applying **mu** (see also Section I.2.2) to a **uc** water retention curve.

Table 9: HYPROPS input file for Example 2.2.

```

-3,7
4
r,0.0,0.3          Set 1 (bc hydraulic
1                  conductivity
1,0.1,bc,1,0.25,0  and bc water
1                  retention)
1,bc,0.05,0.25,0
g,0.0,0.3          Set 2 (bc hydraulic
1                  conductivity
1,0.1,bc,1,0.25,0  and uc water
1                  retention)
1,uc,0.05,0.25,0
b,0.0,0.3          Set 3 (mu hydraulic
1                  conductivity
1,0.1,mu,1,0,0     and bc water
1                  retention)
1,bc,0.05,0.25,0
i,0.0,0.3          Set 4 (mu hydraulic
1                  conductivity
1,0.1,mu,1,0,0     and uc water
1                  retention)
1,uc,0.05,0.25,0

```

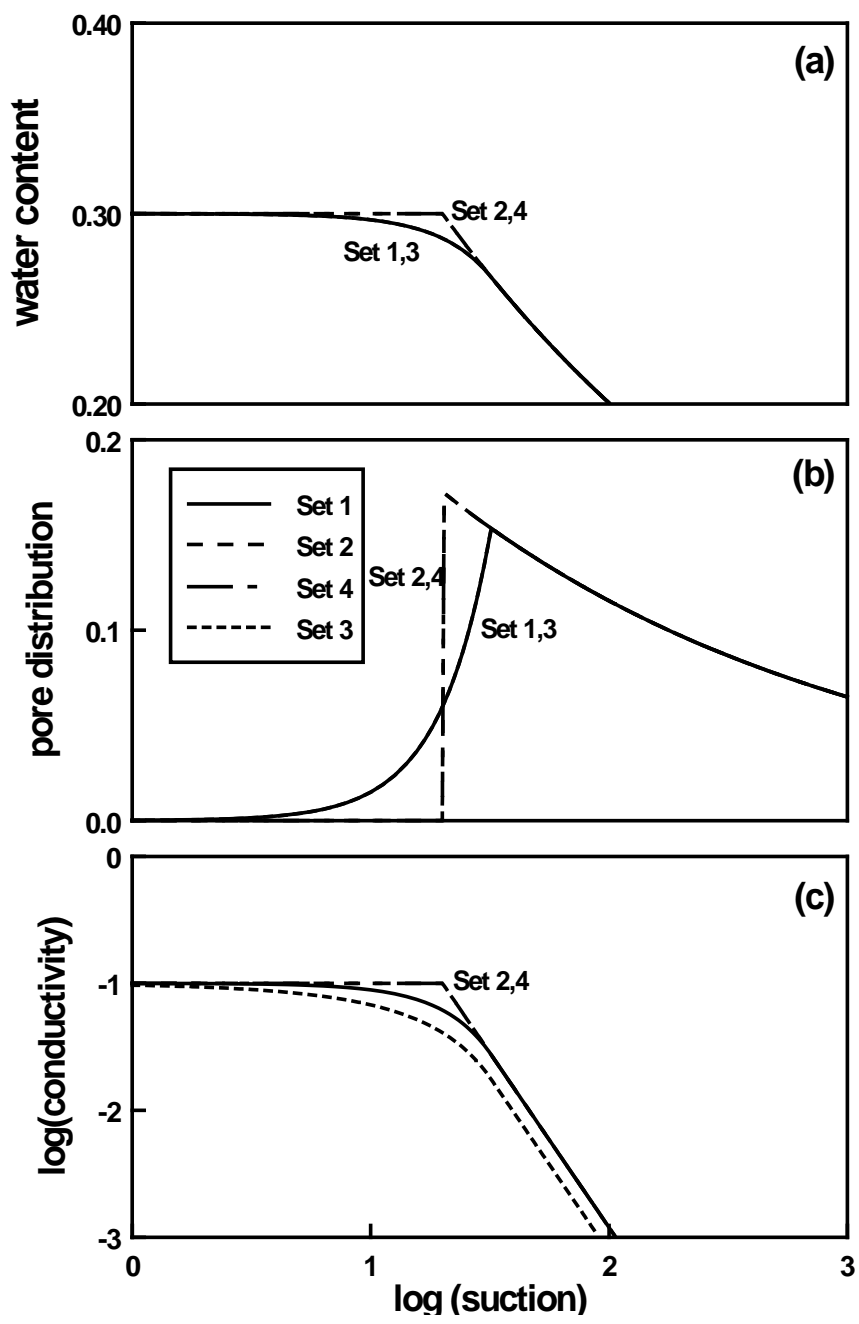


Figure 21: (a) water retention curves, (b) pore-size distributions, and (c) hydraulic conductivity functions for the four cases (Set 1-4, see Table 9) of Example 2.2. Set 2 and 3 are not visible in (a) and (b), because they overlap with Set 4 and 1, respectively. In (c) Set 2 is identical to the Set 4.

Example 2.3

The effect of summing several simple functions is shown in Fig. 22. Here two pore-space distributions are chosen such that they do not overlap in terms of the representative pore sizes (Set 1 and 2 in Fig. 22b). Set 3 and 4 in Fig. 22 combine the properties of Set 1 and 2, by defining each as a component (see input file in Table 10). The weighting factors for the water retention curve and pore size distribution plot are given by the cfrac parameters (compare Eq. (32) in Section I.2.2 and Table 10). These weighting factors do not affect the position of the hydraulic conductivity curve. Even though the cfrac parameters have different values, the hydraulic conductivity functions are the same for Set 3 and 4. The total (summed) hydraulic conductivity function only depends on K_{si} (compare Eq. (31) in Section I.2.2). Note that the Set 2 is not strictly speaking a soil type described by one water retention curve (**ex**) (Table 10). The **ex** water retention curve cannot be used on its own and always needs to be defined in conjunction with some other function. As the aim of this example was to illustrate the summing of functions in Fig. 22, the fractional contribution of the term (tfrac) with the **bc** function was set very low, so that its effect would be minimal at small matric potentials.

Table 10: HYPROPS input file for Example 2.3.

```

-3,7
4
r,0.0,0.3          Set 1 (matrix properties
1                  - mu and bc)
  1,0.1,mu,1,0,0
  1
    1,bc,0.05,0.25,0
g,0.0,0.3          Set 2 (macropore
1                  properties -
  1,10,mu,1,0,0    mu and ex; bc
2                  is added because
  0.001,bc,0.05,0.25,0 ex cannot be
  0.999,ex,4.3,0,0  used on its own)
b,0.0,0.3          Set 3 (matrix and
2                  macropore
  0.5,0.1,mu,1,0,0  properties; each
  1                  contributing 50%
    1,bc,0.05,0.25,0 to overall water
  0.5,10,mu,1,0,0  retention curve)
  1
    1,ex,4.3,0,0
i,0.0,0.3          Set 4 (matrix and
2                  macropore
  0.1,0.1,mu,1,0,0  properties; the
  1                  macropores
    1,bc,0.05,0.25,0 contribute 90%
  0.9,10,mu,1,0,0  to overall water
  1                  retention curve)
    1,ex,4.3,0,0

```

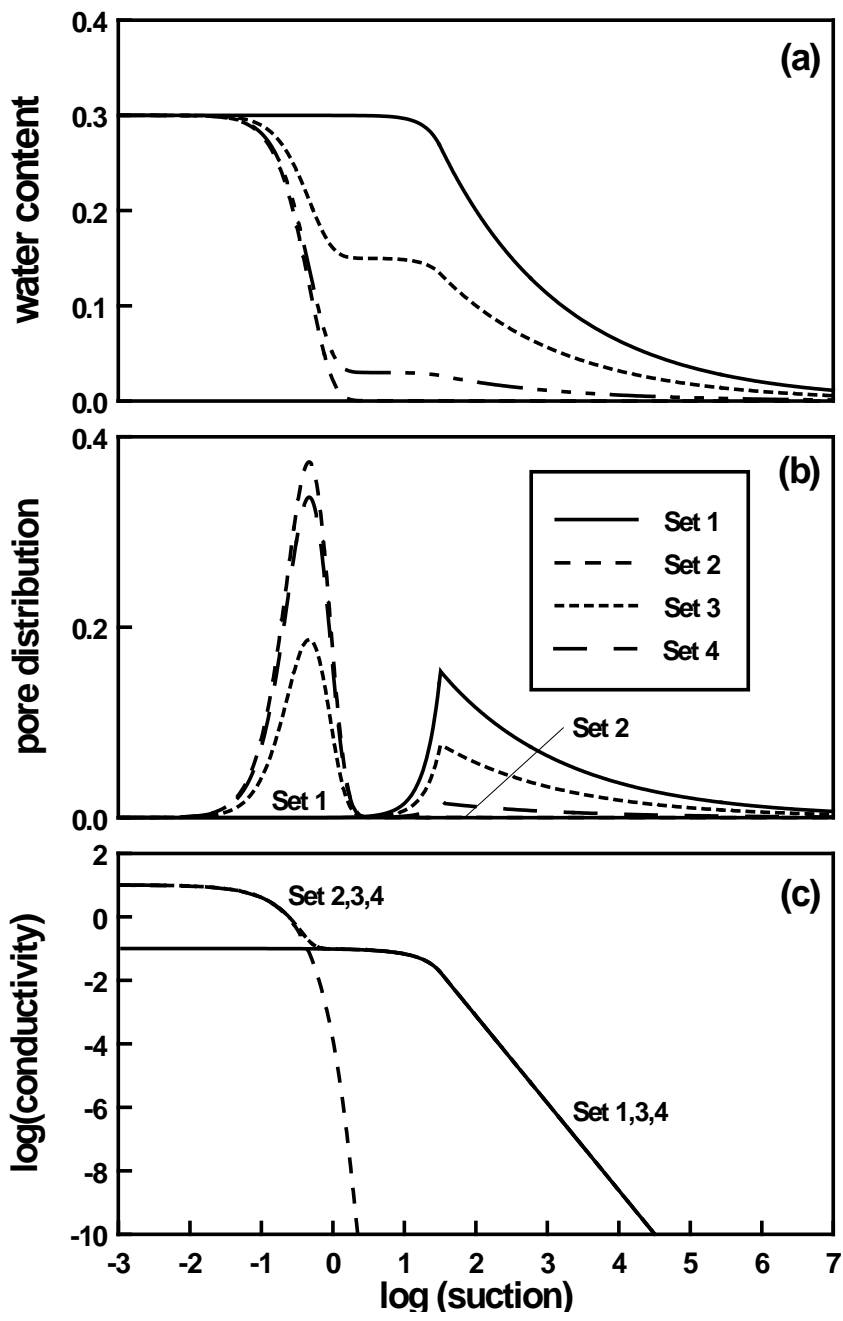


Figure 22: (a) water retention curves, (b) pore-size distributions, and (c) hydraulic conductivity functions for the four cases (Set 1-4, see Table 10) of Example 2.3. In (c), Set 3 is identical to Set 4 and both overlap partly with Set 1 (dry end) and partly with Set 2 (wet end).

Example 2.4

If the macropores present in a soil are sparsely distributed, they do not significantly contribute to the water retention curve, but may still have a large effect on the hydraulic conductivity near-saturation (Smettem and Ross, 1992; Clothier and Smettem, 1990). This effect can be simulated by HYPROPS. In this case the water retention curve associated with macropore component is effectively cancelled out by setting its cfrac to zero (Table 11, Fig. 23a,b). This does not affect the contribution of this component to the hydraulic conductivity function as shown in Fig. 23c. The water retention curve still needs to be defined though, as it is used in the description of the hydraulic conductivity function (compare Eq. 25, 27, 28, 29, 30).

Table 11: HYPROPS input file for Example 2.4

-3,7	
3	
r,0.0,0.3	<i>Set 1 (matrix properties</i>
1	<i>- mu and bc)</i>
1,0.1,mu,1,0,0	
1	
1,bc,0.05,0.25,0	
g,0.0,0.3	<i>Set 2 (macropore</i>
1	<i>properties -</i>
1,10,mu,1,0,0	<i>mu and ex; bc</i>
2	<i>is added because</i>
0.001,bc,0.05,0.25,0	<i>ex cannot be</i>
0.999,ex,4.3,0,0	<i>used on its own)</i>
b,0.0,0.3	<i>Set 3 (matrix and</i>
2	<i>macropore</i>
1,0.1,mu,1,0,0	<i>properties; sparse</i>
1	<i>macropores do</i>
1,bc,0.05,0.25,0	<i>not contribute to</i>
0,10,mu,1,0,0	<i>the water</i>
1	<i>retention curve)</i>
1,ex,4.3,0,0	

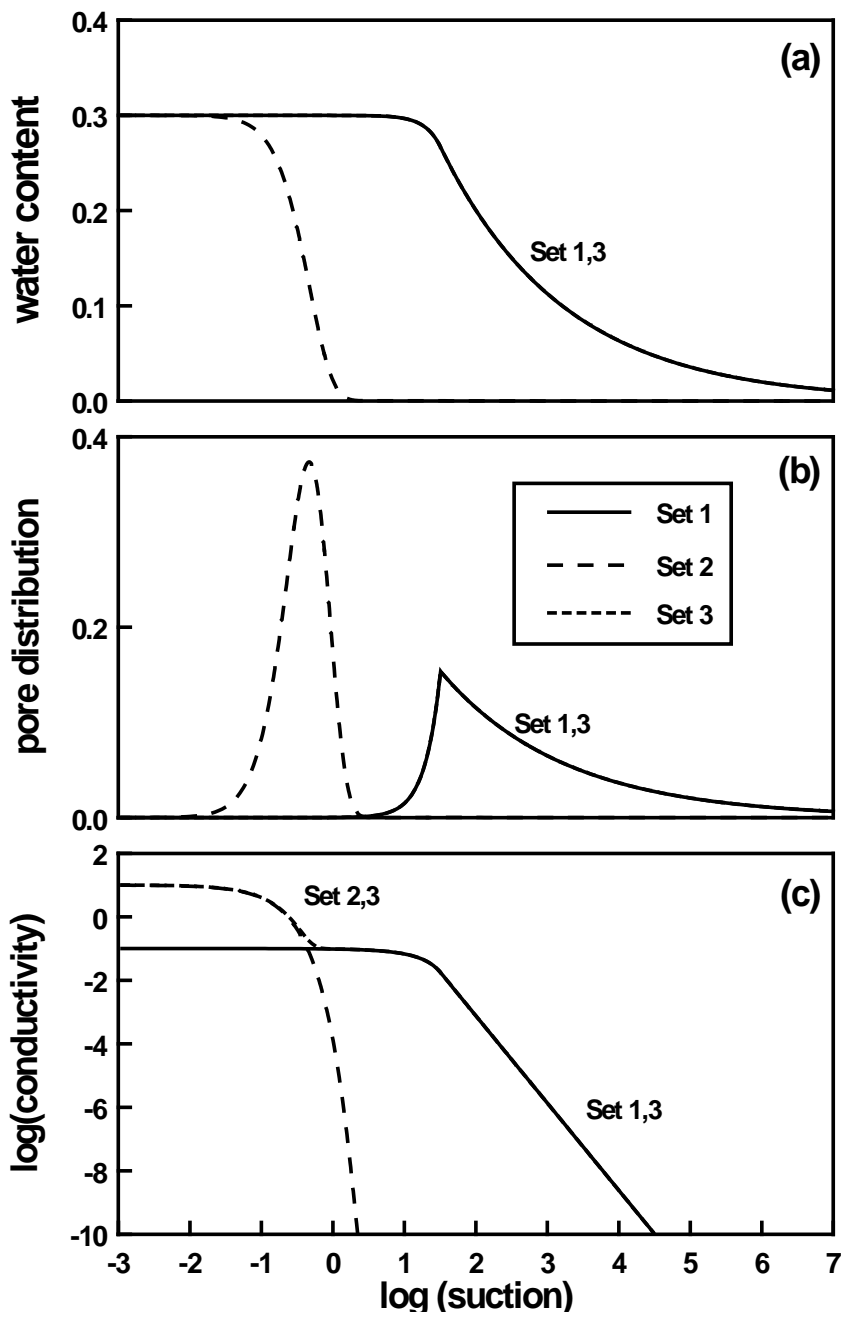


Figure 23: (a) water retention curves, (b) pore-size distributions, and (c) hydraulic conductivity functions for the three cases (Set 1-3, see Table 11) of Example 2.4. Set 3 is not visible in (a) and (b) because it overlaps with Set 1. In (c) it overlaps partly with Set 1 (dry end) and partly with Set 2 (wet end).

Example 2.5

Table 12 gives the equivalent parameterisations of the SWIMv2.1 and SWIMv1 models for a case where an extra macropore component is added to the hydraulic conductivity function. As the extra macropore component only affected the hydraulic conductivity function in SWIMv1, this is achieved by adding a component of which the water retention curve is cancelled out by setting cfrac to zero (Fig. 24a, Table 13). The shape of the hydraulic conductivity function is, however, different from that in Example 2.4.

Table 12: Equivalent parameterisation of SWIMv2.1 and SWIMv1.

SWIMv2.1	SWIMv1						
b,0.0,0.3	thetas	psie	b	Ks	n	Km	m
2	0.3	-20	4	0.1	0	10	12.5
1,0.1,bc,1,0.25,0							
1							
1,bc,0.05,0.25,0							
0,10,bc,40,0.25,0							
1							
1,bc,0.05,0.25,0							

Table 13: HYPROPS input file for Example 2.5

-3,7	
3	
r,0.0,0.3	<i>Set 1 (matrix properties</i>
1	<i>- bc and bc)</i>
1,0.1,bc,1,0.25,0	
1	
1,bc,0.05,0.25,0	
g,0.0,0.3	<i>Set 2 (macropore</i>
1	<i>properties -</i>
1,10,bc,40,0.25,0	<i>bc and bc, but</i>
1	<i>p=40)</i>
1,bc,0.05,0.25,0	
b,0.0,0.3	<i>Set 3 (matrix and</i>
2	<i>macropore</i>
1,0.1,bc,1,0.25,0	<i>properties; sparse</i>
1	<i>macropores do</i>
1,bc,0.05,0.25,0	<i>not contribute</i>
0,10,bc,40,0.25,0	<i>to the water</i>
1	<i>retention curve)</i>
1,bc,0.05,0.25,0	

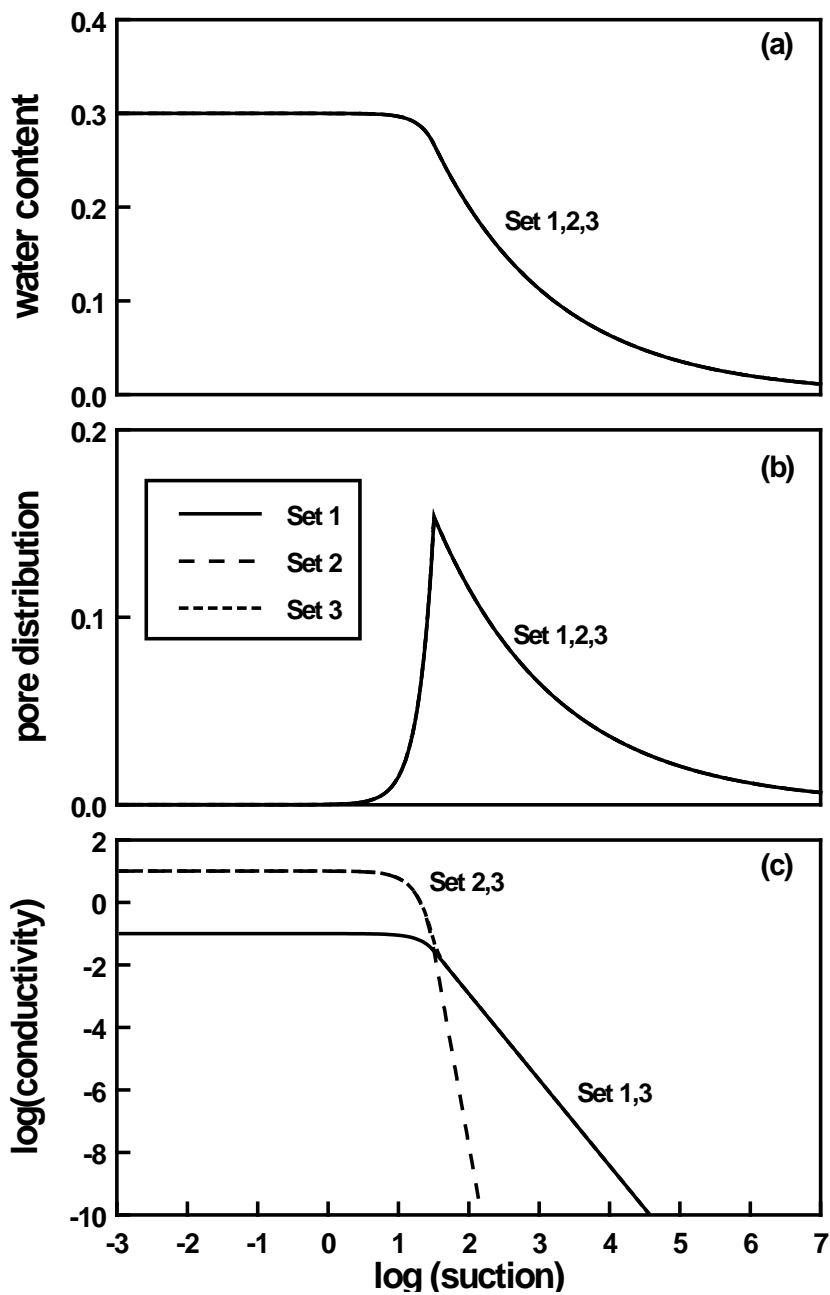


Figure 24: (a) water retention curves, (b) pore-size distributions, and (c) hydraulic conductivity functions for the three cases (Set 1-3, see Table 13) of Example 2.5. Set 2 and 3 are not visible in (a) and (b) because they overlap with Set 1. In (c) Set 3 partly overlaps with Set 1 (dry end) and partly with Set 2 (wet end).

3. USING SWIMPLOT TO VIEW THE OUTPUT OF SWIMv2.1

The SWIMPLOT program uses the binary output file from SWIMv2.1, to show graphically the movement of water and solute with time. The input file to SWIMv2.1 must have been parameterised with “input file for swim v2.1@” for SWIMPLOT to work (first line of input file, see Section II.1.2). The program was written by Steve Bailey and Peter Ross (CSIRO Division of Soils, Townsville)

3.1 Running SWIMREAD

To use the SWIMPLOT program, type the following command line in the DOS environment:

```
swimplot
```

The program will then ask for an input file which is the file *filename.out* generated by SWIMv2.1.

The speed of the SWIMPLOT show can be chosen by the user (keys 0-9) and the output can be temporarily stopped by toggling the “P” key. Pressing the “D” key results in printing of the screen. Note that this does not work successfully with all printers. The screen can also be captured in file. For this purpose press Alt+PrintScrn and paste the clipboard picture into a painting program. Press the “Q” key to quit the program before it has finished.

An example of the screen during the SWIMPLOT run is shown in Fig. 25.

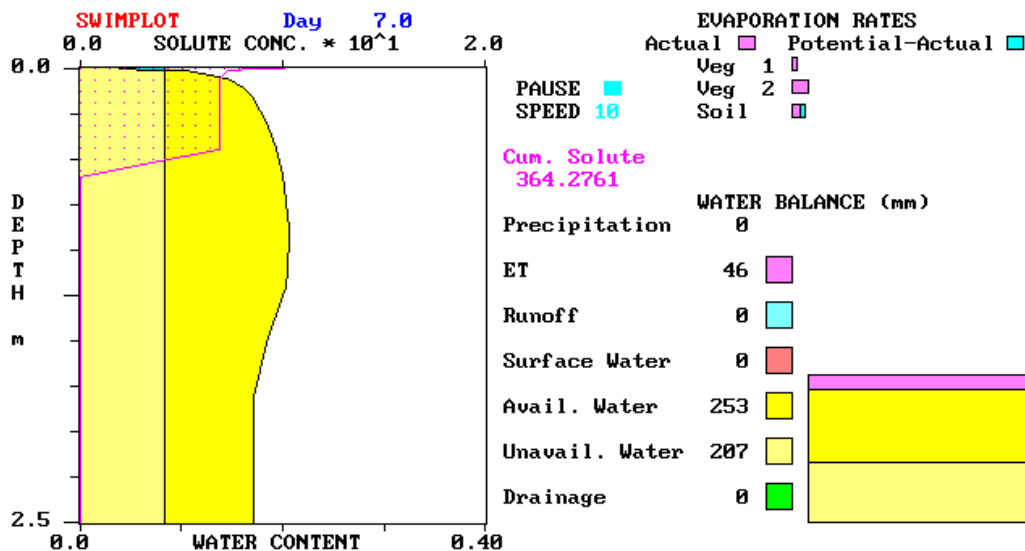


Figure 25: Example of a screen during SWIMPLOT show.

4. USING SWIMREAD TO CREATE TABLES OF OUTPUT DATA

The SWIMREAD program reads the SWIMv2.1 binary output file and compiles ASCII tables of output data. The files can then be imported into spreadsheets and graphics packages like EXCEL, Lotus123, Lotus Freelance and Grapher. The program was developed by Warren Bond (CSIRO Division of Soils, Canberra).

4.1 Running SWIMREAD

To use the program, type the following command line in the DOS environment:

```
swimread filename.out format.inr
```

Here *filename.out* is the binary output file of SWIMv2.1 and *format.inr* is a file that specifies which data will be extracted. The file *sample.inr*, that is provided with the program, is an example of such a file.

4.2 Preparing the input file for SWIMREAD

The first line of the format file (*format.inr*) defines whether the output time units are hours or days (see Example in Section II.4.3). The subsequent lines contain the identifiers of the various types of data that are to be extracted (each on a new line). All possible identifiers and their descriptions are given in Table 14 below, but as few as one can be used. The identifiers will generate separate ASCII files with the corresponding extensions, as given in the table. Three output identifiers call for further information to be given. These are:

drain and leach - these identifiers expect a minimum of one line following them: the first line indicates the number of depths at which the outputs are required; if this is 0, all possible depths are assumed and no further information is required; if the first line is not equal to 0, a second line of list directed input is required, listing the depths at which the output variable is required;

pro - this identifier generates profiles at given times, resulting in an output that is essentially the same as the console output, at each of the specified times. A list of the times (in the units specified at the start of the input file) is required to follow the pro identifier; the number of times is not required. Please note that the pro identifier and list of times should appear at the end of the input file.

Table 14: SWIMREAD format options

property	identifier	file
water content	theta	<i>filename.th</i>
water potential	psi	<i>filename.psi</i>
gradient	grad	<i>filename.grd</i>
water flux	flow	<i>filename.flo</i>
cumulative water flux	drain	<i>filename.dra</i>
solute concentration (solution)	csol	<i>filename.cso</i>
solute concentration (total)	ctot	<i>filename.cto</i>
solute flux	sflo	<i>filename.sfl</i>
cumulative solute flux	leach	<i>filename.lea</i>
water balance	wbal	<i>filename.wbl</i>
profiles at given times	pro	<i>filename.pro</i>

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III - APPENDICES

1. LIST OF KNOWN SWIM REFERENCES

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4. LIST OF SYMBOLS

a	= constant in bc and mc water retention equation [-]
a	= central weighting extension factor [-]
a	= constant in tortuosity Eq. 55 [-]
a	= constant in kinetic energy equation
a	= constant in simple power law runoff function (roff0)
a	= constant in tortuosity equation[-] (a)
a_1	= constant in sigmoid relative growth function
a_2	= constant in sigmoid relative growth function
A	= area of water flow [cm^2]
b	= constant in tortuosity Eq. 52 [-] (dthc)
b	= constant in tortuosity Eq. 55 [-]
b	= constant in Brooks-Corey equations [-]
b	= constant in kinetic energy equation
b	= constant in simple power law runoff function (roff1)
b_1	= constant in sigmoid relative growth function
b_2	= constant in sigmoid relative growth function
B_i	= given by Eq. (82) [cm]
c	= solute concentration in solution [μmol or μg solutes / cm^3 water]
c	= constant in bc and mc water retention equation [$1/\text{cm}^2$]
c_v	= soil vapour concentration [cm^3/cm^3]
c_v'	= saturation vapour concentration [cm^3/cm^3]
d	= $d\psi/dp$ [-]
dt	= timestep [t]
D	= combined dispersion and diffusion coefficient [cm^2/h]
D_v	= vapour diffusivity in the soil [cm^2/h]
D_0	= ionic or molecular diffusion coefficient in free water [cm^2/h] (d0)
E	= evaporation rate [cm/h]
E	= cumulative rainfall energy [J/cm^2]
E_{cr}	= energy in an amount of rain equal to the given hrc falling at 2.5 cm/h [J/m^2]
E_{cs}	= energy in an amount of rain equal to the specified grc falling at 2.5 cm/h [J/cm^2]
E_{ff}	= effectiveness parameter [-]
E_p	= potential evaporation rate [cm/h]
f	= density distribution function [-]
f	= sigmoid relative growth function [-]
f_v	= flux density of vapour flow [cm/h]
g	= $-dz/dx$ (gravity factor) [-]
g	= gravitational constant ($9.8 * 10^2$) [cm/s^2]
g	= defined in Eq. (26)
g_r	= root conductance [$\text{cm}^2/\text{h}/\text{cm}$ root] (groot)
G	= conductance of the seal [1/h]
G_{bp}	= conductance [1/h]
$G_{initial}$	= initial seal conductance [1/h] (g1)
G_{min}	= minimum seal conductance [1/h] (g0)

h	= main drying curve
h	= relative humidity [-]
h	= heigh of ponded water [cm]
h_a	= relative humidity of the atmosphere above the soil [-] (hair)
h_s	= relative humidity at the soil surface [-]
h_0	= depth of water on the surface when runoff just starts [cm]
$h_{0initial}$	= initial surface storage [cm] (hm1)
h_{0min}	= minimum surface storage [cm] (hm0)
H	= hydraulic head [cm]
I	= rainfall intensity [cm/h]
I_r	= standard rainfall intensity (2.5) [cm/h]
k	= coeff. Freundlich isotherm [(mol adsorbed solute/g soil)/(mol solute/cm ³ water) ^{η}] (k)
k_v	= defined by Eq. (41) [cm/h]
K	= hydraulic conductivity [cm/h]
K_r	= relative hydraulic conductivity [-]
K_s	= saturated hydraulic conductivity [cm/h]
K_{s0}	= hydraulic conductivity in bulk soil [cm/h]
KE	= kinetic energy per unit precipitation [J/cm ² /cm rain]
KE_r	= kinetic energy per unit precipitation for $I_r = 2.5$ cm/h [J/cm ² /cm rain]
l	= length of root [cm]
L_i	= root length density of layer i [cm root/cm ³ soil]
L_0	= slope length [cm] (roff1)
m	= constant in vg equations [-]
m	= constant in Eq. (34) [-]
M	= number of components [-] (nc)
M	= molecular weight of the undissociated solute [g/mol = $\mu\text{g}/\mu\text{mol}$]
\overline{M}	= weighted average ionic weight of all species present [g/mol = $\mu\text{g}/\mu\text{mol}$]
M_w	= mass of one mole of water (0.018) [kg/mol]
n	= constant in vg equations [-]
n	= Manning's roughness coefficient [-] (roff0)
n	= constant in dispersion equation [-] (disp)
n	= constant in Brooks-Corey hydraulic conductivity fucntions Eq. (33), (34), and (77)
N	= number of terms [-] (nterms)
p	= hyperbolic sine transform [cm]
p	= pore interaction index [-]
Pe	= Peclet number [-]
q	= water flux density = vol. water flow per unit cross-sectional area per unit time [cm/h]
q	= runoff rate [cm ² /s]
q_{bp}	= bypass flux [cm/h]
q_L	= potential downslope flux density [cm ³ /cm ² /h]
Q	= rate of water uptake by root [cm ³ /h]
r	= radial distance from the root axis [cm]
r	= hydraulic radius [cm]
r_r	= root radius [cm] (rad)
r_{s0}	= radial distance in soil [cm]

r_v	= boundary layer and aerodynamic resistance [(kg/m ²)/(cm/h)]
r_{KE}	= relative kinetic energy per unit precipitation [-]
R	= gas constant (8.3143 * 10 ⁴) [kg cm ² /s ² /mol /K]
R	= net runoff rate (i.e. rate “off” - rate “on” from upslope) [cm/h]
R_s	= soil resistance [h cm ² /cm ²]
R_r	= root resistance [h cm ² /cm ²]
s	= slope gradient [cm/cm]
s	= adsorbed concentration [μmol/g soil or μg/g soil]
S	= source or sink strength (cm water per cm distance per hour) [1/h]
S	= effective saturation [cm ³ /cm ³]
S_{bp}	= bypass channel storage [cm/cm]
t	= time [h]
T	= absolute temperature [K]
T	= transpiration rate [cm/h]
T_a	= actual transpiration rate [cm/h]
T_{max}	= maximum transpiration rate [cm/h]
T_p	= potential transpiration rate [cm/h]
v	= mean runoff flow velocity [cm/s]
v	= pore water velocity = q/θ [cm/h]
w	= distance in downslope direction [cm]
w_1	= weighting factor [-]
w_2	= weighting factor [-]
x	= distance into the soil [cm]
x	= depth [cm]
x_{ibp}	= depth of bypass node ibp [cm]
x_0	= depth of surface node [cm]
z	= gravitational potential [cm]
z	= fractional distance of between main drying and wetting curves (fh) [-]
gf	= gravity factor (1 for vertical flow) [-]
dh	= shift of wetting curve with respect to drying curve
hyscon	= shape parameter scanning curves
slupf	= factor for solute uptake [-]
grc	= conductance precipitation constant [cm]
hrc	= storage precipitation constant [cm]
α	= constant in vg water retention equation [1/cm]
α	= slope angle (see Fig. 3)
α_{ex}	= constant in ex water retention equation [1/cm]
β	= slope angle (see Fig. 3)
χ	= osmotic coefficient [-]
ε	= dispersivity of the medium [(cm ² /h) / (cm/h) ^{n}] (dis(i))
ε	= fractional contribution of component [-] (cfrac)
ϕ	= solute source/sink term [μmol/cm ³ /h or μg/cm ³ /h]
ϕ	= fraction of function in overall water retention curve [-] (tfrac)
ϕ_{cr}	= solute uptake by the crop [μmol/cm ³ /h or μg/cm ³ /h]

ϕ_p	= solute production in the profile [$\mu\text{mol}/\text{cm}^3/\text{h}$ or $\mu\text{g}/\text{cm}^3/\text{h}$]
η	= power of Freundlich isotherm [-] (fip(i))
λ_1	= first-order decay coefficient for dissolved phase [1/h] ($-\lambda_1 = \mathbf{alpha(i)}$)
λ_2	= first-order decay coefficient for adsorbed phase [1/h] ($-\lambda_2 = \mathbf{beta(i)}$)
ν	= number of particles in solution/molecule of solute [-]
θ	= volumetric water content [cm^3/cm^3]
θ_r	= residual water content [cm^3/cm^3] (thr)
θ_s	= saturated water content [cm^3/cm^3] (ths)
ρ	= soil bulk density [g/cm^3] (rhob)
ρ_{vs}	= vapour density at the soil surface [kg/cm^3]
ρ_{va}	= atmospheric vapour density (i.e. of air above soil surface) [kg/cm^3]
ρ_{vs}'	= saturated vapour density at the soil surface [kg/cm^3]
ρ_w	= density of water ($1.0 * 10^{-3}$) [kg/cm^3]
σ	= space -weighting factor Richards' equation(swt) [-]
σ_s	= space -weighting factor advection-dispersion equation (slswt) [-]
τ	= tortuosity factor [-]
ξ	= empirical constant [-] (dthp)
ψ	= matric potential [cm] ($\psi \leq 0$)
ψ_e	= air entry potential [cm] ($\psi_e \leq 0$)
ψ_i	= parameter in bc and mc water retention equations [cm]
ψ_{ibp}	= positive head in bypass tube [cm]
ψ_o	= osmotic potential [cm]
ψ_r	= potential at root surface [cm]
ψ_{s0}	= matric potential in bulk soil [cm]
ψ_t	= soil total potential [cm]
ψ_x	= xylem potential [cm]
ψ_0	= oven-dry potential [cm]
ψ_0	= reversal point (hysteresis) [cm]
ψ_0	= hyperbolic sine transform factor [cm]
ψ_1	= hyperbolic sine transform factor [cm]
ψ_1	= intersection scanning curve and main curve (hysteresis) [cm]
Δx_i	= thickness of layer i [cm]