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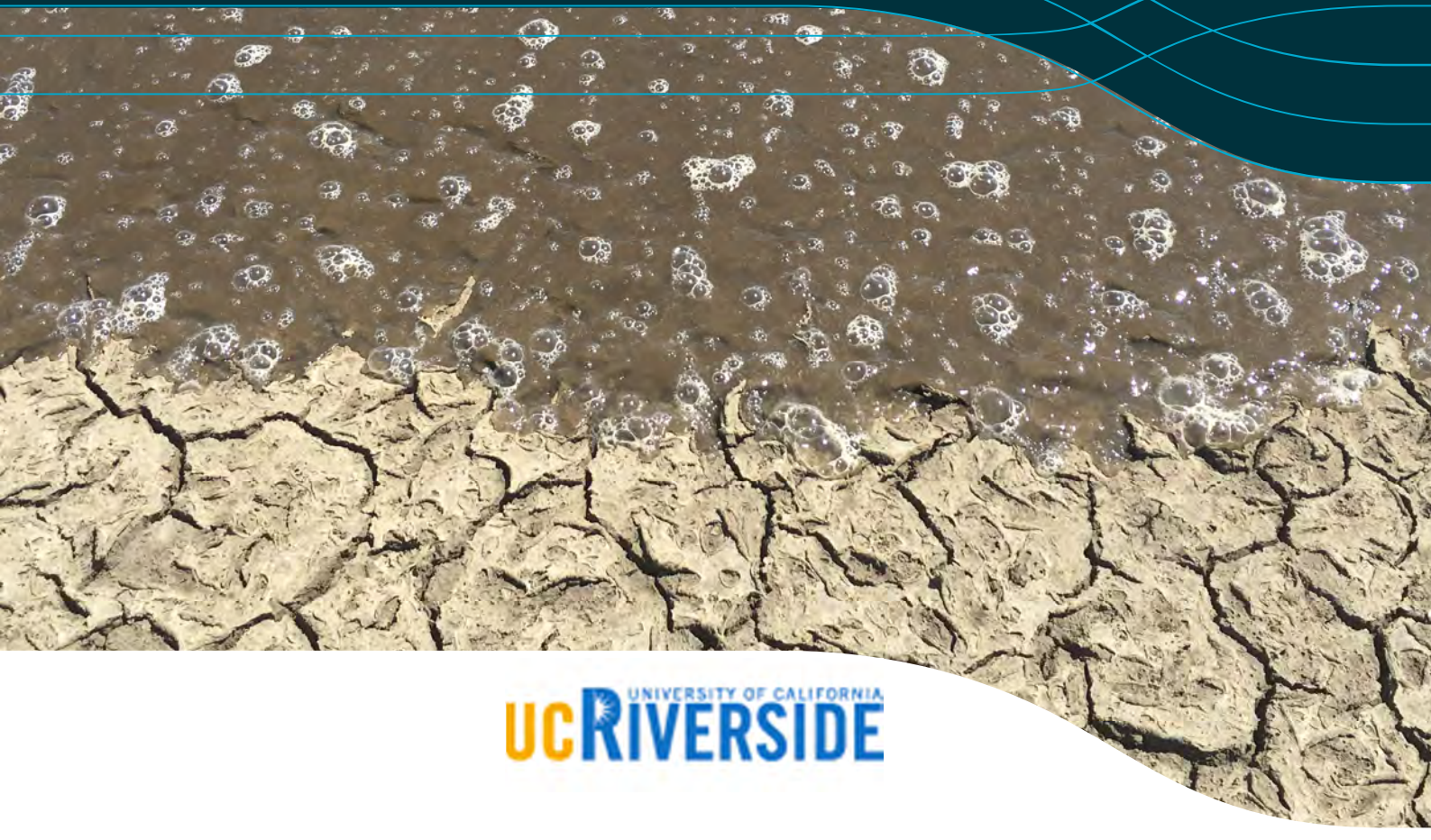
The HYDRUS-1D Software Package for Simulating the One-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media: Tutorial

Version 1.00, July 2018

David Rassam, Jirka Šimůnek, Dirk Mallants,
and
Martinus Th. van Genuchten



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Important disclaimer

This report documents version 4.16 of HYDRUS-1D, a software package for simulating water, heat and solute movement in one-dimensional variably-saturated media. The software has been verified against a large number of test cases. However, no warranty is given that the program is completely error-free. If you do encounter problems with the code, find errors, or have suggestions for improvement, please contact:

Jirka Šimůnek
Department of Environmental Sciences
University of California Riverside
Riverside, CA 92521
USA
Phone/Fax: (951) 827-7854
Email: Jiri.Simunek@ucr.edu

Preface

This tutorial provides a series of example problems for version 4.16 of HYDRUS-1D, a software package for simulating water, heat and solute movement in one-dimensional variably saturated media. The community of HYDRUS users has been growing steadily over the years as evidenced in part by the number of downloads (over 10,000 times each of the past several years) and visits to the HYDRUS web pages at https://www.pc-progress.com/ (on average several hundred each day). The objective of this introductory HYDRUS-1D tutorial is to give HYDRUS-1D users a first hands-on experience with the HYDRUS-1D software package and to familiarize themselves with the overall organization of the HYDRUS-1D graphical user interface, including the main input and output dialog windows. Example problems include variably-saturated water flow in single- and multi-layered soil profiles with and without root water uptake. Both short- and long-term climatic boundary conditions are considered, with a focus on calculating soil water balance and groundwater recharge. Subsequent examples deal with basic advective-dispersive solute transport without solid-liquid interactions, as well as more advanced contaminant transport problems involving linear or non-linear equilibrium sorption reactions and chemical non-equilibrium processes described using one-site sorption kinetics. Physical non-equilibrium (mobile-immobile water type) solute transport is also discussed, as well as the combined effect of physical and chemical non-equilibrium effects on solute transport (i.e., a mobile-immobile type model with two-site sorption in the mobile zone). Two inverse modelling examples consider one-step and multi-step outflow, respectively. The final example is about coupled heat movement and reactive solute transport. All examples can be downloaded from the HYDRUS website (https://www.pc-progress.com/en/Default.aspx?H1d-tut-TutorialBook).

Additional supporting information is provided in an extended Appendix, which is based on Frequently Asked Questions (FAQs) previously discussed on the HYDRUS-1D website. This tutorial provides complementary information to the existing HYDRUS-1D Technical Manual (Šimůnek et al., 2008) and the more theoretical background documentation on soil physical processes implemented in HYDRUS-1D as documented by Radcliffe and Šimůnek (2010). A comprehensive overview of recent developments and applications of the HYDRUS-1D software packages is available from Šimůnek et al. (2016).

CONTENTS

Introduction

This tutorial provides a series of example problems for version 4.16 of HYDRUS-1D, a software package for simulating water, heat and solute movement in one-dimensional variably saturated media. The software consists of several computation modules such as the standard direct module (h1d_calc.exe), the standard inverse module (h1d_clci.exe), a dual-permeability direct module (h1d_dual.exe), a dual-permeability inverse module (h1d_dlin.exe), the UnsatChem module for major ion chemistry and transport (h1d_unsc.exe), and the HP1 module for multicomponent transport (hp1.exe), as well as the HYDRUS-1D interactive graphics-based user interface.

The standard HYDRUS-1D module numerically solves the Richards equation for variably-saturated water flow and advection-dispersion type equations for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The flow equation may also consider dual-porosity type flow in which one fraction of the water content is assumed to be mobile and another fraction immobile, or dual-permeability type flow involving two mobile regions, one representing the matrix and one the macropores or fractures. The heat transport equation considers transport due to conduction and convection with flowing water. Coupled water, vapor, and energy transport can be considered as well. The solute transport equations consider advective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equations also include provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions: one which is independent of other solutes, and one which provides the coupling between solutes involved in sequential first-order decay reactions. In addition, physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual-porosity type formulation which partitions the liquid phase into mobile and immobile regions. Alternatively, the transport equations include provisions for kinetic attachment/detachment of solute to the solid phase, and thus can be used to simulate the transport of viruses, colloids, or bacteria.

The objective of this introductory HYDRUS-1D tutorial is to give HYDRUS-1D users hands-on experience with the software and to familiarize them with the overall organization of the HYDRUS-1D graphical user interface, including the main input and output dialog windows. Example problems include variably-saturated water flow in single- and multi-layered soil profiles with and without root water uptake. The applications consider both short-term (1 and 30 days) and longer-term (1 year) climatic boundary conditions, with a focus on calculating soil water balance and groundwater recharge. Subsequent examples deal with basic advective-dispersive solute transport without solid-liquid interactions, as well as more advanced contaminant transport considering linear or non-linear equilibrium sorption reactions and chemical non-equilibrium described using one-site sorption kinetics. Physical non-equilibrium (mobile-immobile) solute transport is also discussed, as well as the combined effect of physical and chemical non-equilibrium effects on solute transport (i.e., a mobile-immobile type model with two-site sorption in the mobile zone). Two inverse modelling examples consider one-step and multi-step outflow, respectively. The final example is about coupled heat movement and reactive solute transport. All examples can be downloaded from the HYDRUS-1D website (https://www.pc-progress.com/en/Default.aspx?H1d-tut-TutorialBook).

The following specific examples are considered in this tutorial:

1. Infiltration of water into a single-layered soil profile
2. Infiltration of water into a two-layered soil profile
3. Root water uptake
4. Estimating groundwater recharge
5. Basic solute transport
    - 5a. Solute introduced through a constant flux boundary
    - 5b. Solute introduced through a constant pressure head boundary
    - 5c. Profile with non-zero initial concentration
    - 5d. The effects of solute dispersion
    - 5e. The effects of diffusion

6: Advanced solute transport

- 6a. Equilibrium (instantaneous) linear sorption
- 6b. Equilibrium (instantaneous) non-linear sorption
- 6c. Chemical non-equilibrium one-site sorption
- 6d. Physical non-equilibrium, dual-porosity (mobile-immobile water) media
- 6e. Dual-porosity model with two-site sorption in the mobile zone (physical and chemical non-equilibrium)

7. Inverse modeling
    - 7a. One-step outflow method
    - 7b. Multi-step outflow method
8. Heat and reactive solute transport (with a stagnant boundary condition for volatile chemicals)

Example 1: Infiltration of Water into a Single-Layered Soil Profile

Example Description and Objectives

This example problem involves infiltration of water from a ponded soil surface into a 1-m deep single-layered loam soil. The soil profile is initially unsaturated, having an initial pressure head of -100 cm. Water infiltrates from the saturated soil surface, which is represented by a 'Constant Pressure Head' boundary condition by assuming that the pressure head at the soil surface is 1 cm (corresponding to the ponding depth). Water drains from the bottom of the soil profile by gravity (represented by a 'Free Drainage' boundary condition) since the groundwater table is at an unspecified point deep in the profile (e.g., more than 10 m). This introductory example demonstrates the advance of the wetting front throughout the soil profile, examines surface and bottom fluxes, run-time information (such as time steps and a number of iterations), mass balances, and other input and output information.

Pre-Processing

Project Manager

The first step when working with any HYDRUS-1D project involves opening the **Project Manager** (Fig. 1.1) by clicking on the **Project Data Manager** Tab in the upper left corner (third button from the left) of the displayed Graphical User Interface (GUI). The **Project Manager** is a tool to manage data of existing projects and helps to locate, open, copy, delete and/or rename desired projects or their input or output data. A project represents any particular problem to be solved using HYDRUS-1D. The project name, as well as a brief description of the project, helps to locate a particular problem. Input and output data for each project are placed in a folder with the same name as the project. Projects are represented by a file *project_name.h1d* and the *project_name* folder.

The current version of the **Project Manager** gives you considerable freedom in organizing your projects. The projects are grouped into **Work Groups**, which can be placed anywhere in accessible memory (such as on local and/or network hard drives). The **Work Groups** can be any existing accessible subdirectory (folder). HYDRUS-1D is installed together with four default workspaces: *Direct*, *Inverse*, *Unsatch*, and *HP1*, which are located in the HYDRUS-1D folder. The *Direct* and *Inverse* work groups contain test examples for direct and inverse problems, respectively, while the *Unsatch* and *HP1* work groups contain examples for carbon dioxide/major ion chemistry and HP1 biogeochemical examples, respectively. We suggest that you create your own **Work Groups** (e.g., the *My Direct* and *My Inverse* Work Groups) and keep the pre-programmed examples intact for future reference. Projects can be copied with the **Project Manager** only within a particular Work Group. However, you can copy projects between Work Groups using standard file managing software, e.g., Windows Explorer. In that case, you must copy both the folder of a particular project and the *project_name.h1d* file. Another way of copying a project between **Work Groups** is first to open the project, and then using the command **Save As** (File menu) to save that project to a new location.

The **Project Manager** has two Tabs (in the upper left corner): **Project Groups** and **Projects**. The **Project Groups** Tab displays currently defined Project Groups, and the **Project** Tab displays projects in a selected particular Project Group. The **Project Manager** can be obtained either from the File Menu (the command Project Manager) or the Toolbar (the third button).

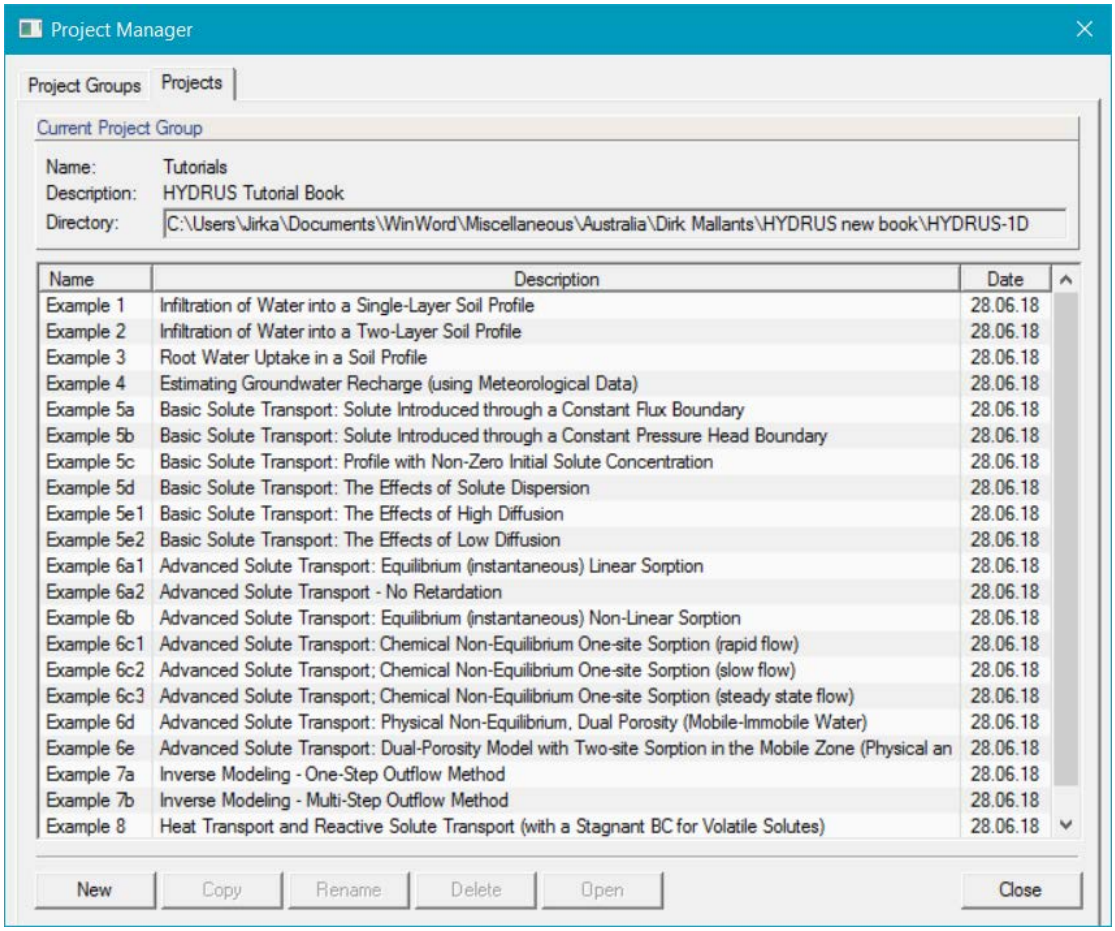

Figure 1.1. The **Project Manager** dialog window.

- Open the **Project Manager** (from the File Menu or the third button on the Toolbar,).
- Select the *Projects* Tab of the Project Manager.
- Click button “New” and the New Project dialog window (Fig. 1.2) will open. This command allows you to create a new project with a given name, provides a brief project description, and indicates where the project files will be located.
- Type the **Name** of the project: “Example 1”
- Type the **Description** of the project: “Infiltration of water into a soil profile”.
- Click button “OK”. A default HYDRUS-1D project is now created, presumably for simulating water flow in a one-dimensional 1-m deep soil profile. This default project now can be modified for a specific problem.

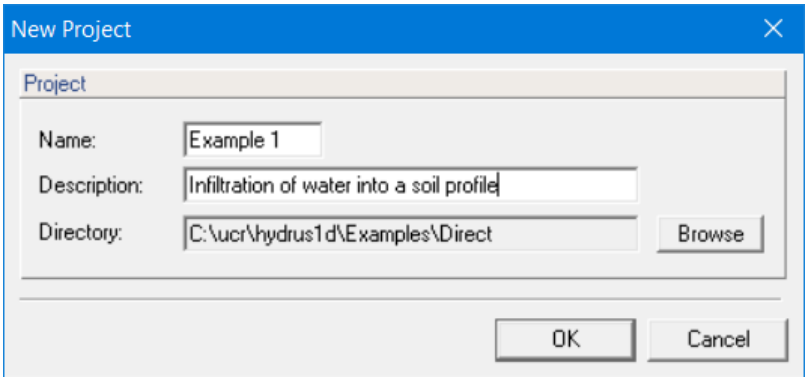

Figure 1.2. The **New Project** dialog window.

Main Processes

Figure 1.3 shows the **Main Processes** dialog window, which is the first window you will encounter when starting a new project. This window will show the processes that can be selected for a particular simulation. When selecting **Water Flow** (see the mathematical description in Chapter 2 of the Technical Manual[1] (Šimůnek et al., 2008)), you can also consider *Vapor Flow* and accumulation/melting of *Snow* at the soil surface. When selecting **Solute Transport,** you can either use the Standard Solute Transport module (Chapter 3), the more specialized Major Ion Chemistry module (Chapter 6), or the biogeochemical module HP1 (which resulted from coupling HYDRUS-1D with the PHREEQC biogeochemical code (Jacques and Šimůnek, 2005; Jacques et al., 2006, 2018)). Because degradation and other transport and reaction processes are temperature dependent (usually degradation increases with temperature), one can also consider **Heat Transport** (Chapter 4) and the effects of temperature on solute reactions (such as contaminant degradation (EFSA, 2008) and organic matter decomposition (Jacques et al., 2018)). When plants are present, one should also consider **Root Water Uptake** and **Root Growth** (Chapter 2.2 and 3.5). The UnsatChem module can be used to simulate carbon dioxide transport (considering diffusion in both liquid and gas phases and convection in the liquid phase) and production (**CO2 Transport**) (Chapter 5), as well as major ion solute transport (Chapter 6). Finally, you can select whether HYDRUS-1D should be run in for a forward prediction, or in the **Inverse Mode** (Chapter 9), in which case various parameters can be calibrated against experimental data and/or experimental data can be displayed together with the simulation results.

- Type Heading: “Infiltration of water into a soil profile”
- Click the *Button* “Next” (or press **n** of the keyboard)

From this point on the program will navigate you through the entire process of entering input information. Users may either select particular commands from a menu (or the pre-processing part of the desktop) or allow the interface to lead them through the process of entering input data by selecting the **Next** button. Alternatively, clicking the **Previous** button will return users to the previous window (since the **Main Processes** dialog window is the first window, the **Previous** button is not present).

[1] Subsequent references to a particular Chapter refer to the HYDRUS-1D Technical Manual (Šimůnek et al., 2008). Much of the information can be accessed immediately also by simply pressing F1, or by clicking on the “Help” button (and then, among other options, clicking on “Help on …” and dragging “?” to a particular pre- or post-processing part of the window).

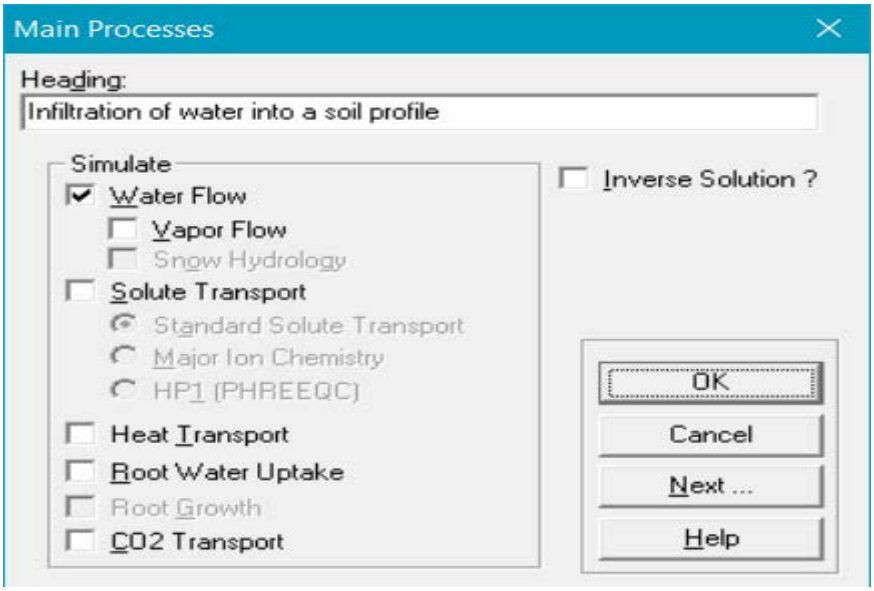

Figure 1.3. The **Main Processes** dialog window.

Geometry Information

The second dialog window one encounters is called **Geometry Information** (Fig. 1.4). In this window, one selects the **Length Unit** (mm, cm, or m), the **Number of Soil Materials** that are present in the system (i.e., the number of soil horizons), the **Number of Layers** over which a **Mass Balance** will be calculated, whether flow is vertical or horizontal (i.e., a **Decline from Vertical Axis** of 1 indicates flow in a vertical direction, while 0 indicates flow a horizontal direction), and the **Depth of the Soil Profile**. Note that when the **Length Unit** is changed later, all input parameters for a particular project will be converted automatically from the original units into the new units.

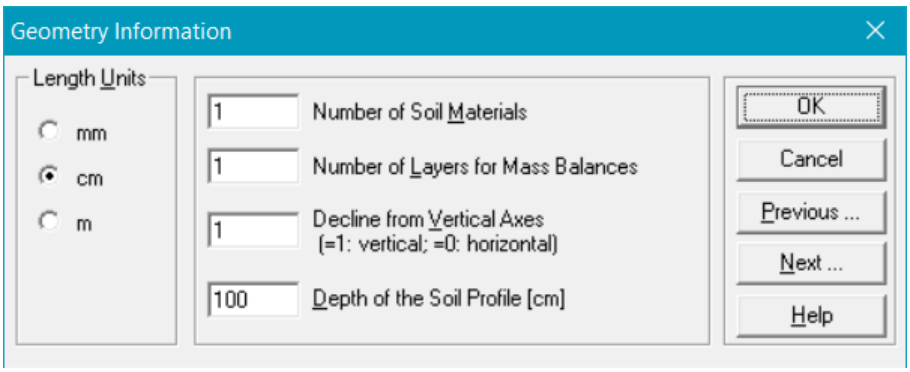

Figure 1.4. The **Geometry Information** dialog window.

- Length Units: cm
- Number of Soil Materials (typically corresponding to the soil horizons): 1 (indicates a homogenous soil profile). The maximum allowed number is 100.
- Number of Layers for Mass Balance: 1 (you may select up to 10 mass balance layers; the default option is a single mass balance layer, which corresponds to the entire soil profile. You may wish to assign individual mass balance layers to

each soil material (horizon) or a group of soil materials, or apply separate mass balances the root zone and the remainder of the soil profile.)
- Decline from vertical axis: 1 (vertical flow)
- Depth of the Soil Profile (cm): 100 cm
- Click *Button* "Next"

Time Information

The third dialog window users encounter is called **Time Information** (Fig. 1.5). Here you select the **Time Unit** to be used throughout the application (i.e., years, days, hours, min, or sec), when the simulation starts (**Initial Time**) and ends (**Final Time**), and how the time should be discretized (i.e., **Initial**, **Minimum**, and **Maximum Time Step**s). We recommend to simply use the default parameters for time stepping in most applications. The boundary conditions will either be constant in time, or one can specify **Time-Variable** Boundary Conditions, such as daily values of precipitation, evaporation, and transpiration. Evapotranspiration fluxes additionally can be evaluated from various **Meteorological Data** using the **Penman-Monteith** combination **equation** recommended by FAO (Monteith, 1981, 1990) or the **Hargreaves Formula** (Jensen et al., 1997). Time-variable boundary conditions can be either constant during specified time intervals or be subject to **Daily Variations** (of transpiration or meteorological data) to be **Generated by HYDRUS-1D** using predefined interpolation functions. Finally, a surface **Energy Balance** can be evaluated from specified meteorological data. Further details on temporal discretization can be found in Appendix I.

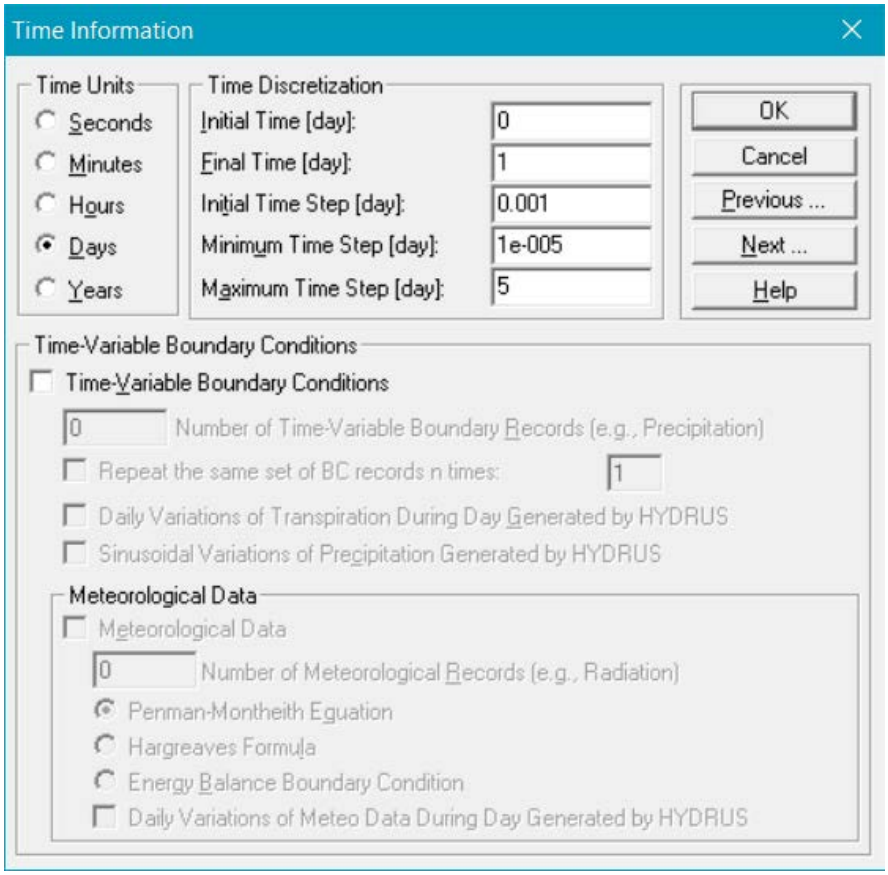

Figure 1.5. The **Time Information** dialog window.

- Time Units: Days
  Time Discretization:
- Initial Time (day): 0
- Final Time (day): 1
- Initial Time Step (day): 0.001
- Minimum Time Step (day): 0.00001
- Maximum Time Step (day): 5 (you do not need to change this even though it is larger than the final time).
- Click *Button* "Next"

Print Information

The fourth dialog window HYDRUS-1D is called **Print Information** (Fig. 1.6). In this window, you simply select how often the output of the model should be printed. Output can be printed at every n^{th} **Time Step** (if 1 then after each time step), at a predetermined **Regular Time Interval**, or at specified **Print Times**, which then will be specified in the next dialog window.

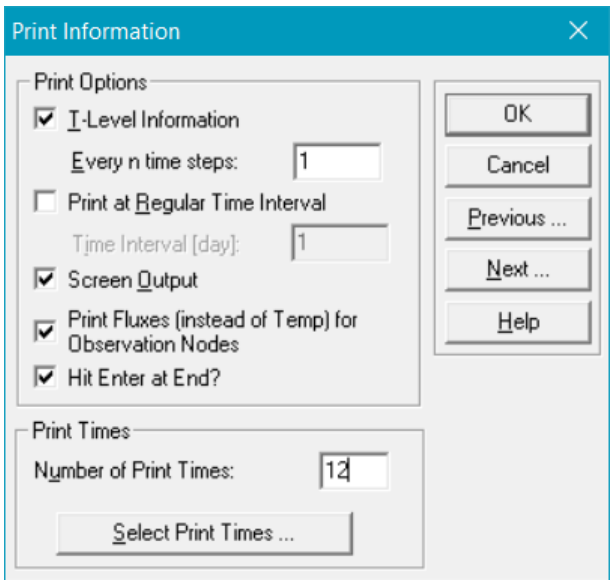

Figure 1.6. The **Print Information** dialog window.

- Print Options: Leave as Default
- Number of Print Times: 12
- Click *Button* "Select Print Times." This command will open a **Print-Times** dialog window (Fig. 1.7), which by default will list uniformly distributed Print Times at which detailed information about pressure heads, water contents, concentrations, water and solute fluxes, and soil-water and solute balances will be printed. These default **Print Times** can be edited as needed. Clicking on the **Default** command button will cause the print times to be distributed evenly between the initial and final time. Clicking on the **Default (log)** command button will cause the print times to be distributed between the initial and final time evenly on a log scale. This option is recommended only for larger times. When using this **Default (log)** option, the first **Print Time** is often extremely small. One should make sure that the Initial and **Minimum Time Steps** (in the **Time Information** dialog window) are smaller than this first Print Time.

- Click *Button* “Next”

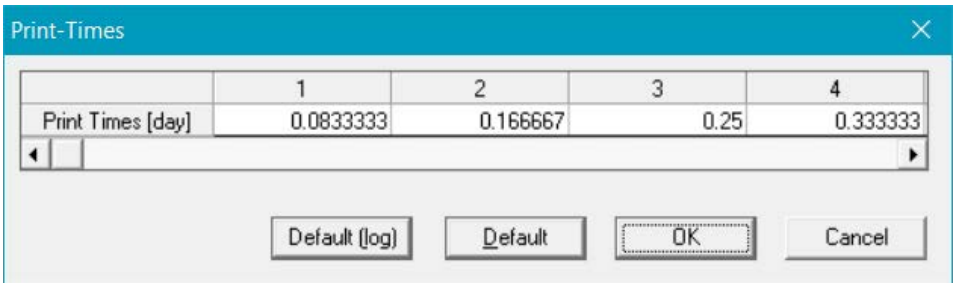

Figure 1.7. The **Print-Times** dialog window.

The first four windows are general windows (with general information), which you need for any application of HYDRUS-1D. All of the dialog windows to be discussed next deal with a) water flow, b) heat transport, c) solute transport, d) root water uptake, and/or other information.

Water Flow – Iteration Criteria

The **Iteration Criteria** dialog window is used to specify iteration criteria, which are required for the numerical solution of the Richards equation (the equation governing water flow in the unsaturated zone) and various **Time Step Control** factors, which depend on the numerical solution (Fig. 1.8). In general, one should not change any of these values, which control the fully automated self-adjusting time-stepping procedure of the numerical solution. The default values are based on many years of experience using the HYDRUS models and their predecessors for a range of applications. More details about iteration criteria and time step control can be found in Appendix I.

Internal Interpolation Tables of water contents, hydraulic conductivities, and specific water capacities are generated from the specified set of unsaturated soil hydraulic parameters. Values of the hydraulic properties are then computed for all numerical nodes during the iterative solution process using linear interpolation between the entries in these tables. This interpolation approach was found to be much faster computationally than direct evaluation of the hydraulic functions over the entire range of pressure heads. Interpolation tables can be avoided by setting both the **Upper** and **Lower Limits of the Tension Interval** to zero. To avoid problems with the numerical solution, the **Internal Interpolation Tables** should not be used when the dual-porosity model of Durner (1994) is used to describe the soil hydraulic functions since this model does not have a monotonous hydraulic capacity function. When the Brooks and Corey (1964) model is used, either the lower limit should be larger (in absolute value) than $1/\alpha$ (i.e., the air-entry value) or the tables should be avoided altogether (e.g., by fixing the lower and upper limits at zero).

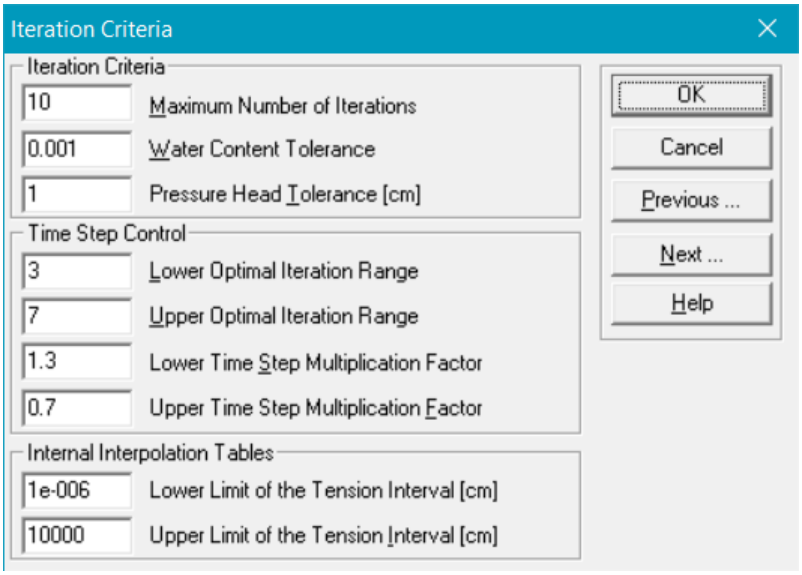

Figure 1.8. The **Iteration Criteria** dialog window.

- Leave default values
- Click *Button* "Next"

Water Flow – Soil Hydraulic Model

HYDRUS-1D allows you to consider different analytical models to describe the soil hydraulic properties (i.e., water retention and hydraulic conductivity functions). The unsaturated soil hydraulic properties can be described in HYDRUS-1D using Brooks and Corey (1964), van Genuchten-Mualem (van Genuchten, 1976), modified van Genuchten (Vogel and Císlerová, 1988), Durner (1994), and Kosugi (1996) type analytical functions. The different analytical models can be selected in the **Soil Hydraulic Model** dialog window (Fig. 1.8). They are described in detail in Chapter 2.4 of Šimůnek et al. (2008) and summarized further in Appendix III. Or, alternatively, you can click on F1 for more information.

The **Soil Hydraulic Model** window allows you to select additionally various models for simulating nonequilibrium or preferential flow, such as dual-porosity or dual-permeability models as summarized by Šimůnek and van Genuchten (2008), and whether or not to consider hysteresis. Hysteresis is a property of soils to have different wetting and drying branches of the soil water retention curve, including scanning curves (Luckner et al., 1989; Lenhard and Parker, 1992; Vogel et al., 1996). One may further limit hysteresis to only the soil water retention curve, or also consider hysteresis in the unsaturated hydraulic conductivity (which generally shows less effects of hysteresis when plotted versus water content)

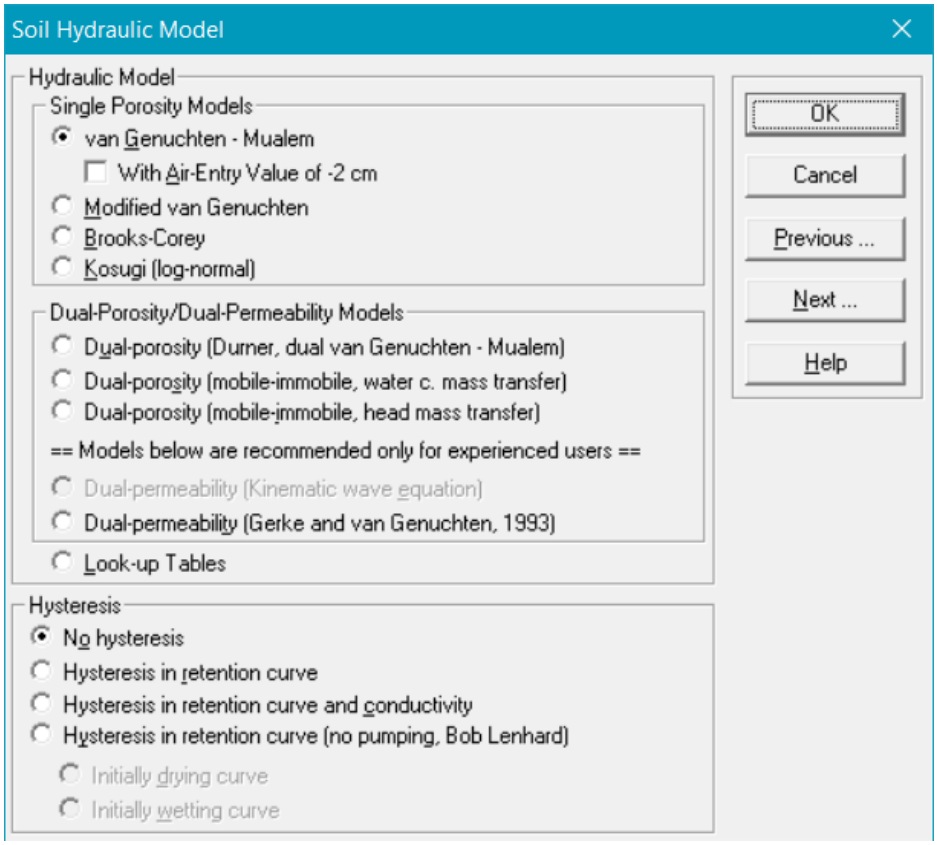

Figure 1.9. The **Soil Hydraulic Model** dialog window.

- Leave as Default (Single Porosity, Models, van Genuchten – Mualem)
- Click *Button* "Next"

Water Flow – Soil Hydraulic Parameters

The **Soil Hydraulic Parameters** for the hydraulic property model selected in the previous dialog window can be specified in the dialog window shown in Figure 1.11.

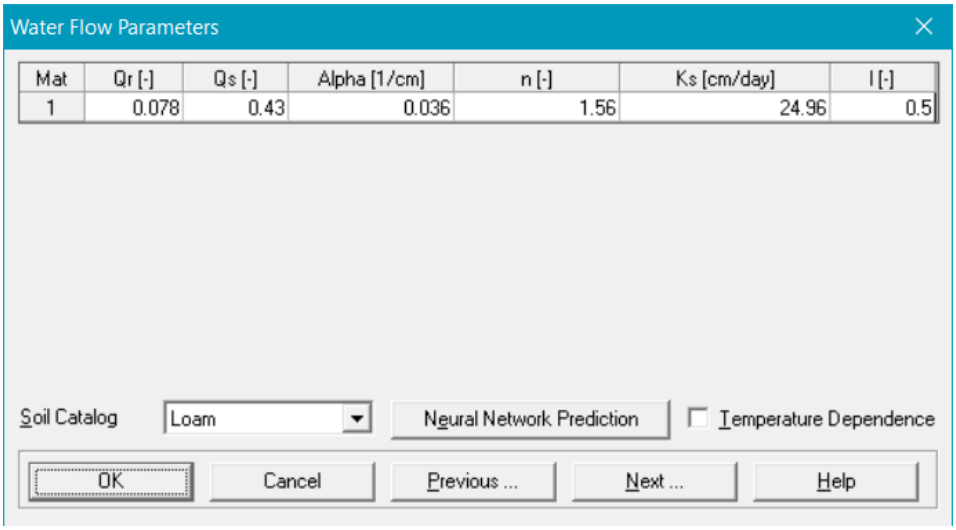

Figure 1.10. The **Water Flow Parameters** dialog window.

It is always preferable to use soil hydraulic parameters based on actual measurements, for example by analyzing observed soil water retention and/or hydraulic conductivity data using the RETC code (van Genuchten et al., 1991), which can be downloaded from the HYDRUS website. Unfortunately, this is not possible when data are limited or lacking. For this reason, we implemented in the **Water Flow Parameters** window a **Soil Catalog,** which provides average soil hydraulic parameters for twelve different USDA soil textural classes as derived by Carsel and Parrish (1988). One can open the **Soil Catalog** and simply select the desired soil texture (which in our current example is actually loam). The hydraulic parameters of that soil type are then immediately transferred to the table in Fig. 1.10. Users should be aware that the average parameters in the **Soil Catalog** were derived for agricultural soils and may not be appropriate for relatively deep soil horizons.

Additionally, we also implemented in the **Water Flow Parameters** window the option of selecting pedotransfer functions, which relate easily measured soil properties such as texture and bulk density with the hydraulic parameters. The pedotransfer functions used in HYDRUS-1D are those developed by Schaap et al. (2001) as incorporated into their Rosetta module (**Neural Network Prediction**; Fig. 1.11). While hydraulic parameters obtained with Rosetta may be superior to those from the **Soil Catalog**, we decided to keep the soil catalog, mostly for historical reasons.

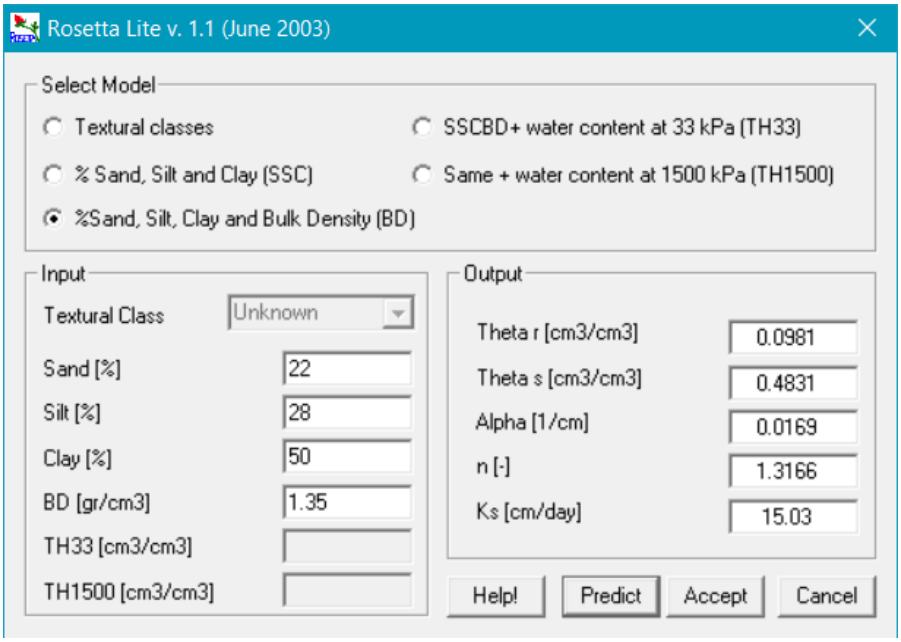

Figure 1.11. The **Rosetta Lite** dialog window.

Finally, the temperature dependence of soil hydraulic parameters can be considered by selecting the **Temperature Dependence** checkbox in the **Water Flow Parameters** window. The influence of temperature on the soil water pressure head is then quantitatively predicted from the effect of temperature on surface tension (Philip and de Vries 1957), while the influence of temperature on the hydraulic conductivity is predicted from the effect of temperature on viscosity and the density of water (Constantz, 1982).

- θ_r (residual water content, units depend on the selected length unit; here cm^3/cm^3)
- θ_s (saturated water content, units depend on the selected length unit; cm^3/cm^3)
- Alpha (the hydraulic shape parameter α, units depend on the selected length unit; here 1/cm)
- n (the hydraulic parameter n, dimensionless)
- K_s (the saturated hydraulic conductivity, units depend on the selected length and time units; here cm/day)
- l (Mualem's pore connectivity exponent; the default value of 0.5 is used here)
- Select Loam from the Soil Catalogue (the default soil texture in HYDRUS-1D)
- Click *Button* "Next"

Water Flow – Boundary Conditions

The **Water Flow Boundary Conditions** window (Fig. 1.12) allows you to select boundary conditions for the top and bottom of the soil profile, depending upon the application More information on the meaning and application of various boundary conditions are found in Appendix II (and/or see Chapter 2.7 or press the F1 key). Various constant or time-variable, pressure heads or water fluxes, as well as atmospheric boundary conditions, can be used at the soil surface. For the bottom of the soil profile, you can additionally select free or deep drainage boundary conditions, a seepage face, or horizontal drain conditions. Additionally, in the **Initial Condition** part of the dialog window, you must specify whether the initial conditions for water flow are to be given later in terms of the pressure head or the water content.

The water table in the current example is assumed to be located far below the bottom of the soil domain and thus does not affect flow processes in the adopted soil profile (e.g., by capillary rise). This default BC (**Free drainage**) corresponds to gravity flow (i.e., flow according to a total unit hydraulic gradient).

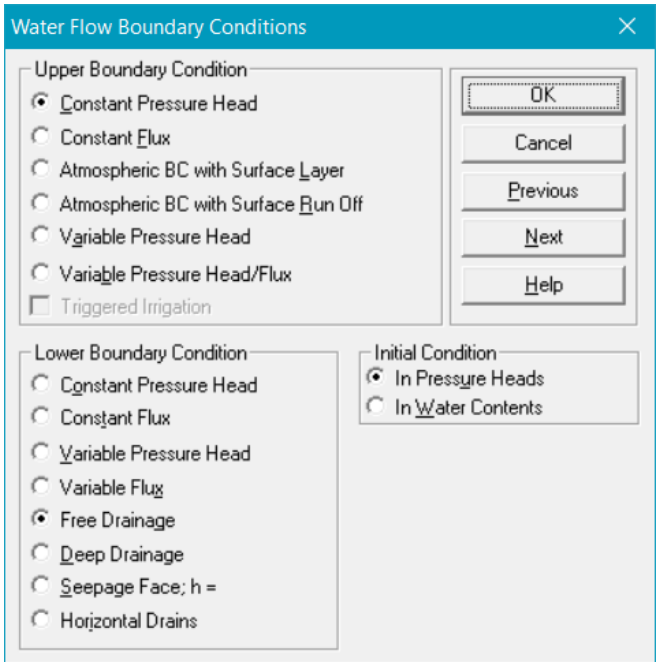

Figure 1.12. The **Water Flow Boundary Conditions** dialog window.

- Upper Boundary Condition: Constant Pressure Head (see Appendix II.1.1)
- Lower Boundary Condition: Free Drainage (see Appendix II.1.7)
- Initial Condition: In Pressure Heads
- Click *Button* "Next"

HYDRUS-1D Guide

The next dialog window (Fig. 1.13) will ask "**Do you want to run PROFILE application?**" When selecting OK, the external **Profile** module, in which users can specify spatially variable properties (such as material distribution, initial conditions, root water uptake distribution, observation nodes, etc.), will be opened.

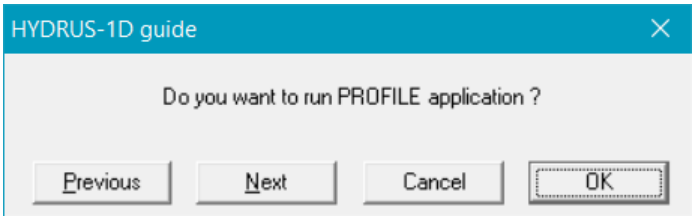

Figure 1.13. The **HYDRUS-1D Guide** dialog window.

- Click *Button* "OK"

At this point, you will get an additional question "**Do you want to save data before running the Graphical Profile Editor?**" Please answer yes since you want the external **Profile** module to reflect the information entered thus far in the main module, such as which processes were selected, what the depth of the soil profile is, and what type of the boundary conditions will be used.

Soil Profile – Graphical Editor

HYDRUS-1D discretizes by default[2] the soil profile into 100 finite elements (FE) involving 101 nodes. Since the profile was assumed to be 100 cm, the elements all have a size of 1 cm. This default discretization is appropriate for this simple example. However, there are other problems for which you may need to refine the FE grid at certain locations along the modeled soil profile. More details on the spatial discretization can be found in Appendix I.

- **Menu**: Conditions->Initial Conditions->Pressure Head, or press the Red Arrow (i.e.,) on the **Toolbar**
- Click the "Edit Condition" *Button* on the left-side Edit Bar, select with your Mouse the top node (the selected node should now have a yellow color), then left-click the mouse again, and specify a pressure head of 1 cm. This is now the top boundary condition corresponding to the ponding depth on the soil surface. Note that when a constant pressure head boundary condition is used, its value is entered into the initial condition and then kept constant during the simulation. All other nodes will remain at the default initial pressure head of -100 cm.

[2] Since the default number of finite elements is always 100, the element size will depend on the assumed total profile length.

- **Menu**: Conditions->Observation Nodes, or press  of the Toolbar
  Note that when you move the cursor around the view window, you can monitor its position, i.e., the node numbers and the depth, at the lower right corner.
- Click the "Insert" *Button* on the left-side **Edit Bar**, and specify nodes at 20, 40, 60, 80, and 100 cm. Use a left click to insert an observation node, and a right-click to end the command (hence you can add several observation nodes after the initial left click).
- Observation nodes can be deleted using the "Delete" and "Delete All" commands of the Edit Bar. In addition to serving as locations for which the output (pressure head, water content, temperature and concentration at each time step) is printed, observation nodes also provide necessary output required for specific applications. For example, observation nodes are used to identify the location of experimental data points used in inverse modeling projects, or the location of a threshold pressure head for triggered irrigation (see Appendix II).
- **Menu**: File->Save Data, or use **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

After exiting the "**Soil Profile**" Editor, the **Soil Profile Summary** dialog window (Fig. 1.14) appears. This window provides tabular information about the spatial discretization ("**z [cm]**"), initial conditions ("**h [cm]**"), spatial root distribution ("**Root [1/cm]**"), scaling factors ("**Axz**", "**Bxz**", "**Dxz**"), and material distributions (**Mat**) with depth, among other data. This table is adjusted automatically to accommodate concentration and temperature data if the solute and heat transport options had been activated in the Main Processes window. In the window, **Axz** is the nodal value of the dimensionless scaling factor α_h [-] associated with the pressure head, **Bxz** is the nodal value of the dimensionless scaling factor α_K [-] associated with the saturated hydraulic conductivity, and **Dxz** is the nodal value of the dimensionless scaling factor α_θ [-] associated with the water content (see Chapter 2.4 or press F1).

The command "**Set to Default Values**", if used, would set all values in this table to its default values. The command "**Set Initial Conditions equal to Field Capacity**" would set the initial values equal to Field Capacity. Field capacity in HYDRUS-1D is defined as the water content or pressure head corresponding to the hydraulic conductivity of about 0.01 cm/d (Twarakavi et al., 2009).

- Click *Button* "Next"

HYDRUS-1D Guide

The next dialog window (Fig. 1.15) will now appear and ask "**Do you want to run HYDRUS-1D application?**" When you select OK, another dialog window appears and asks "**Do you want to save the input data before executing HYDRUS-1D?"**. You should always answer these questions positively by clicking on "**Yes**", except when realizing that some errors may have been made and should be corrected (then click on "**No**"). Once "**Yes**" is chosen, the external computational **H1D_Calc.exe** module will be executed.

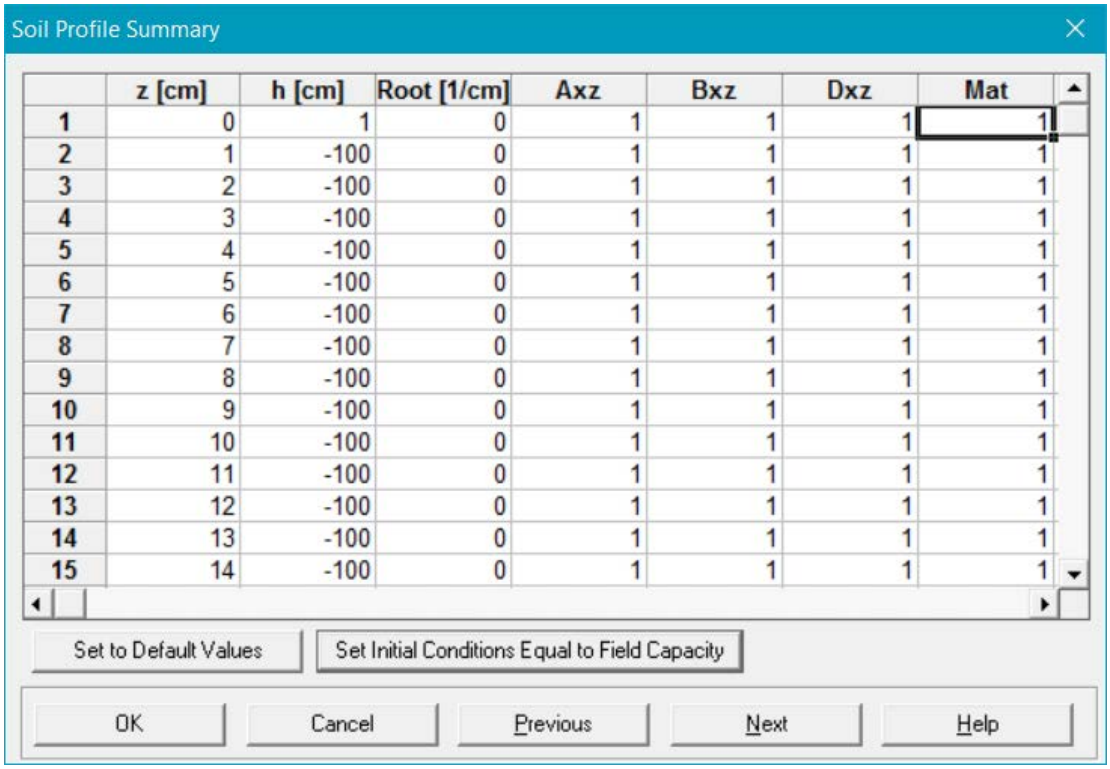

Figure 1.14. The **Soil Profile Summary** dialog window.

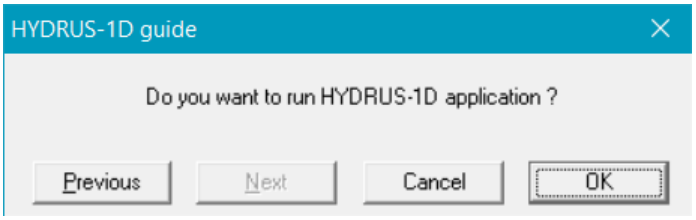

Figure 1.15. The **HYDRUS-1D Guide** dialog window.

- Click *Button* "OK"
- Alternatively, you can run the computational module using the **Menu Command**: Calculation->Execute HYDRUS-1D or a Toolbar button  .

Execute HYDRUS-1D

The computations are now being carried out, with parts of the results being displayed in a DOS window (Fig. 1.16). This window will show selected run-time information, such as time (*Time*), the number of iterations (*ItW*), the cumulative number of iteration (*ItCum*), the surface flux (*vTop*), the cumulative surface flux (*SvTop*), cumulative root water uptake (*SvRoot*), the cumulative bottom flux (*SvBot*), the surface pressure head (*hTop*), the average pressure head in the root zone (*hRoot*), and the bottom pressure head (*hBot*). When the simulation ends, the Run Time in seconds is displayed, as well as the note "Calculations have finished successfully". You are now asked to "*Press Enter to Continue*". Once the keyboard button "Enter" is pressed, the DOS window is closed and the program returns to the HYDRUS-1D GUI. Detailed output information

will not be shown in the DOS window if the user does not check the “Screen Output” box in the Print Information dialogue window.

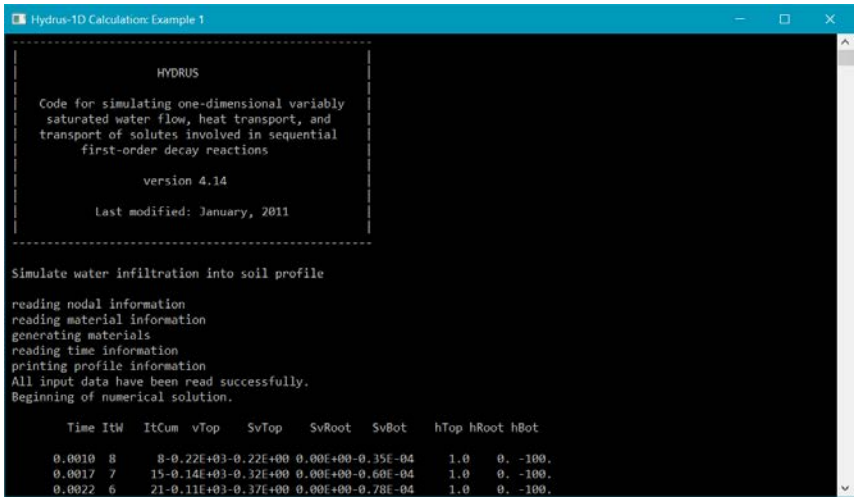

Figure 1.16. The DOS window in which the computational module h1d_calc.exe is executed.

Post-Processing

Once the calculations are finished and the “Enter” button is pressed, the “Post-Processing” section (the right side) of the main window of the HYDRUS-1D GUI will be populated with commands that can be used to display selected results, which will be discussed below ((Fig. 1.17)). Program output consists of a number of output files that are described in detail in Chapter 13 of the technical manual. These output files are located in the project folder, the location of which is indicated in the Project Manager of the HYDRUS-1D GUI. The output files are in standard text format and as such can be opened by any standard text editing programs, such as Notepad or MS Excel.

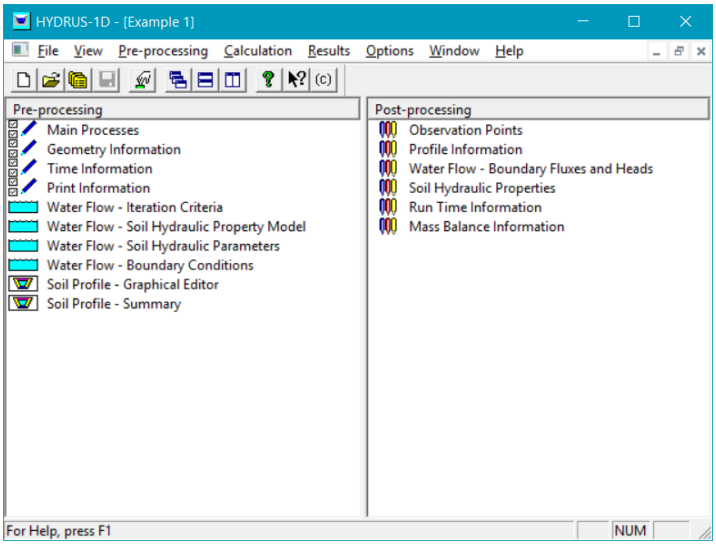

Figure 1.17. The main window of the HYDRUS-1D GUI with both pre- and post-processing commands.

Observation Points

Pressure heads (Fig. 1.18), water contents, and water fluxes at selected observation nodes (i.e., at depths of 20, 40, 60, 80, and 100 cm) are displayed under the command "**Observation Nodes"** at the post-processing section of the HYDRUS-1D GUI (or using the menu command "Results->Observation Nodes).

Referring to Figure 1.18:

- Note how the pressure heads evolve over time at the selected observation points. This output option is useful when one requires the model to produce predictions at a specific location to compare with field observations (such as observed pressure heads from a tensiometer or water contents from a TDR probe) and is particularly relevant when conducting inverse simulations (parameter identification or model calibration).
- Note that the wetting front passes the selected depths of 20, 60, and 100 cm at times of approximately 0.08, 0.35, and 0.65 days, respectively. This timing is dictated by the hydraulic properties of the loam soil.
- When the wetting front approaches a certain depth, the pressure head increases from the initial value of -100 cm and eventually reaches 1 cm (not shown in Fig. 1.18, where the maximum displayed pressure head is zero), which is equal to the imposed positive pressure head at the surface.
- The colors in Figure 1.18 show which curve belong to which node (i.e., N1, N2, …). This connection is not immediately shown initially but appears when you right-click on the figure, select "Legend…", and then click on "Visible". Many other options can be used by right-clicking on the figure, including copying the figure. You can also alter the labels along the axes (e.g., to use different fonts or font sizes), or change the scales of the axes by right-clicking on the axis itself. These changes are possible with all post-processing figures that are generated.

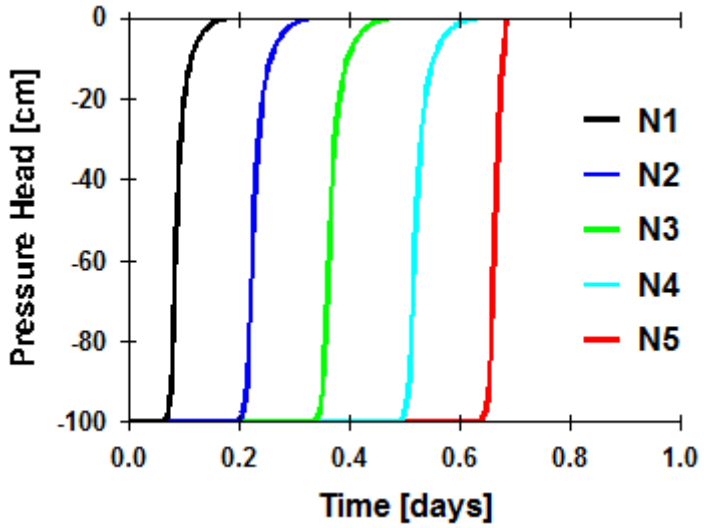

Figure 1.18. Pressure heads versus time at selected observation points (N1 - 20 cm, N2 - 40 cm, N3 - 60 cm, N4 - 80 cm, and N5 - 100 cm).

Profile Information

Pressure heads (Fig. 1.19), water contents (Fig. 1.20), water fluxes, hydraulic conductivities, and hydraulic capacities versus depth at selected Print Times (i.e., every two hours in this example) are displayed using the command "**Profile Information"** of the post-processing section of the HYDRUS-1D GUI (or using the menu command "Results->Profile Information).

- Figure 1.19 shows the advance of the wetting front at selected print times. For example, after 0.08 days (2 hours), the wetting boundary had reached a depth of about 20 cm (similar results are shown in Figure 1.18 for the first observation point N1).
- The wetting front advances in time until it reaches the bottom of the profile at about 0.75 days. The entire profile then attains a pressure head of 1 cm.
- Figure 1.20 portrays the same information for the water content, with the initial water content equal to 0.24 (as defined by the initial pressure head of -100 cm and the soil water retention curve of the loam soil). Note that once the wetting boundary passes a certain point, the water content becomes equal to the saturated water content (θ_s) of 0.43 (see Water Flow Parameters: Qs=0.43).

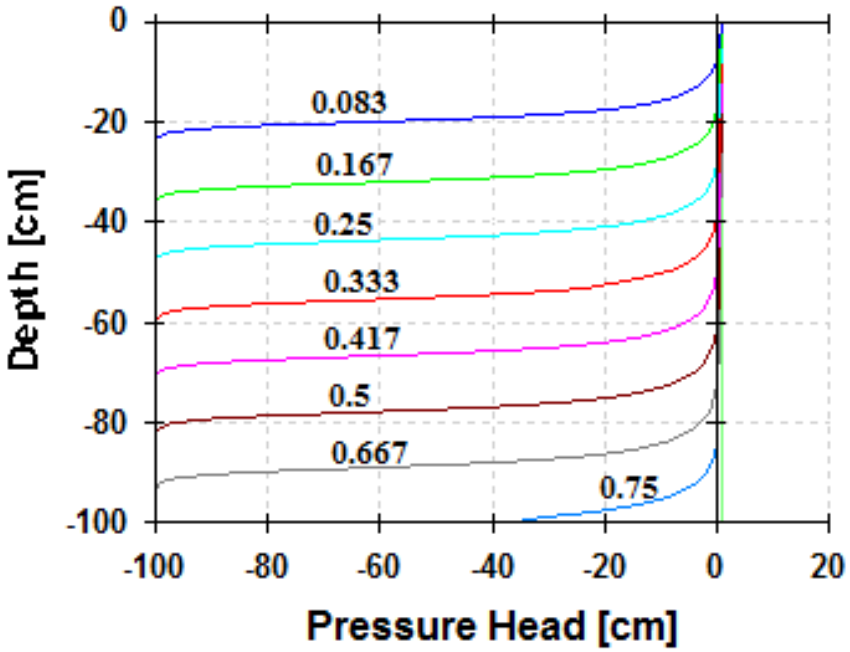

Figure 1.19. Pressure head profiles at selected print times (from 0.083 to 0.75 days).

Water Flow - Boundary Fluxes and Heads

Various water fluxes (potential and actual surface fluxes, potential and actual root water uptake rates, and bottom fluxes, as well as their cumulative values) and pressure heads (at the surface and bottom of the profile, and average root zone pressure heads) versus time are displayed under the command "**Water Flow - Boundary Fluxes and Heads"** of the post-processing section of the HYDRUS-1D GUI (or using the menu command "Results->Water Flow - Boundary Fluxes and Heads") (Fig. 1.21).

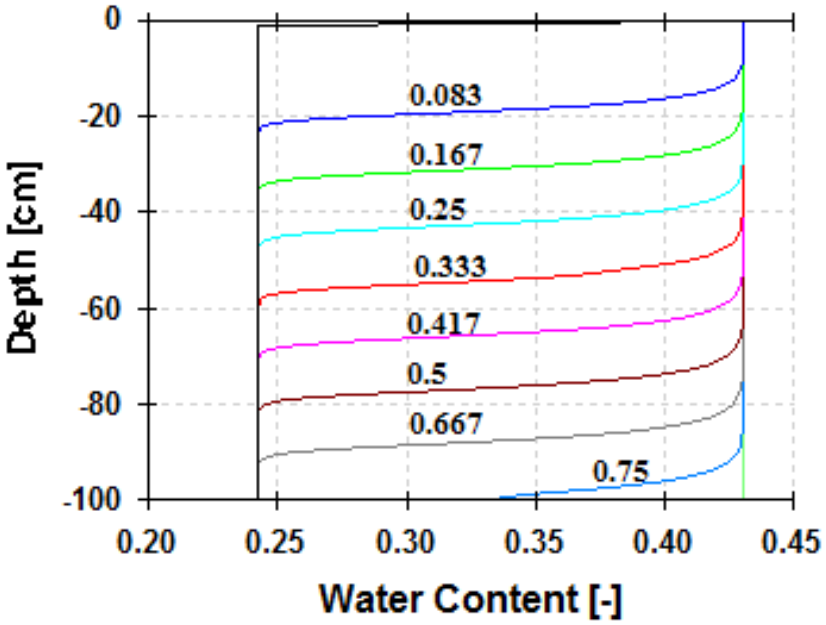

Figure 1.20. Water content profiles at selected times (from 0.083 to 0.75 days).

Referring to Figure 1.21:

- Note that HYDRUS-1D reports downward fluxes (against the direction of the *z*-axis) as negative and upward fluxes (in the direction of the *z*-axis) as positive. This is due to the convention in the numerical solution that the z-axis is positive upward.
- Water starts infiltrating at the soil surface due to the 1 cm positive pressure head imposed at the "Constant Head Boundary" and continues to do infiltrate during the entire simulation.
- The lower "Free Drainage Boundary" allows unit gradient gravity drainage. However, the initial magnitude of this drainage is so small that it does not show in this figure at early times (before the arrival of the wetting front).
- As soon as the wetting front reaches the lower boundary (after about 0.70 days; see also the pressure head profiles in Figure 1.18), the bottom flux increases significantly. Note that the two lines representing the upper and lower boundary fluxes become parallel (i.e., inflow = outflow), and the water balance of the soil profile reaches a steady-state.

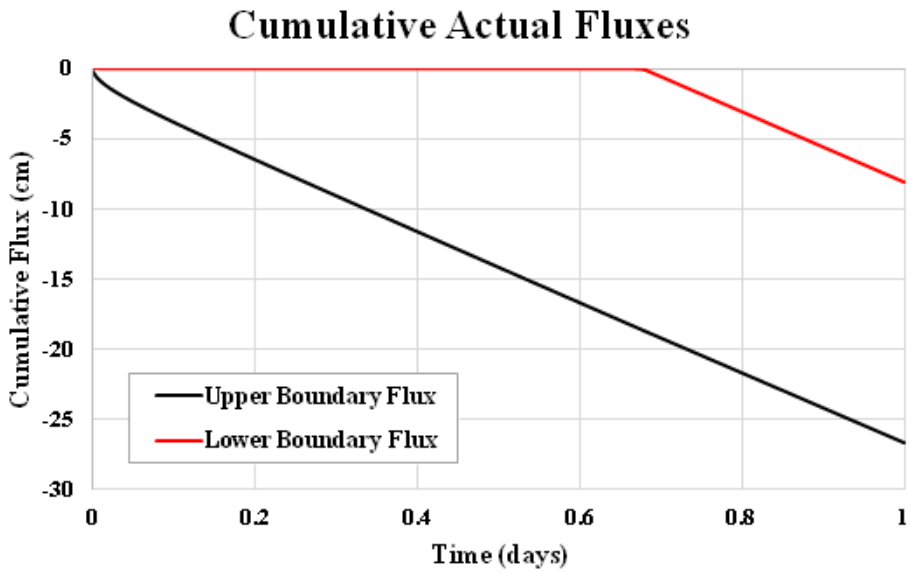

Figure 1.21. The surface flux (negative and into the soil profile) and the bottom flux (negative and out of the soil profile) versus time.

Soil Hydraulic Properties

Graphs of the unsaturated soil hydraulic functions (various combinations of pressure heads, water contents, hydraulic conductivities, and soil water capacities) for soils in the soil profile are displayed using the command "**Soil Hydraulic Properties**" of the post-processing section of the HYDRUS-1D GUI (or using the menu command "Results->Soil Hydraulic Properties") (Fig. 1.22).

- Figure 1.22 shows the water retention curve for the selected "Loam" soil. Note that the horizontal axis is the logarithm of the absolute value of the pressure head, thus representing matric suctions in terms of pF units (one cannot take the logarithm of a negative number). Values of 0, 1, 2, 3, and 4 hence represent pressure heads equal to -1, -10, -100, -1000, and -10,000 cm, respectively). Plots using pF values often provide a better display of the entire soil water retention curve, including values near saturation (such as between -1 and -10 pressure heads in the current example).
- Note from Figure 1.22 that the water content at a pressure head of -100 cm (i.e., pF=log(|h|) = 2), which is the initial condition, is equal to about 0.24. This value of 0.24 is the initial water content in Figure 1.20).
- The "**Soil Hydraulic Properties**" command allows users to view the soil water retention and the hydraulic conductivity functions of the soil or soils being studies, among other combinations of soil hydraulic properties (the list boxes of the commend provide many graphing options, including the use of regular of logarithmic scales).

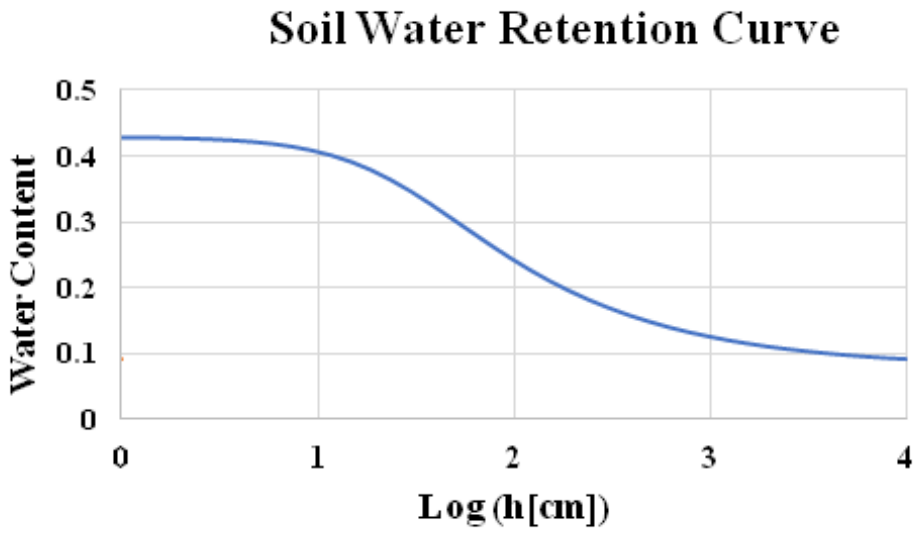

Figure 1.22. Soil water retention curve.

Run Time Information

Selected information about the numerical solution (such as temporal changes in the time step, the number of iterations necessary to solve the Richards equation at any particular time level, the cumulative number of iterations, and the dimensionless Peclet and Courant numbers when solute transport is considered) versus either time or the number of time-steps are displayed under the command "**Run Time Information**" of the post-processing section of the HYDRUS-1D GUI. One could for this purpose use the menu command "Results->Run Time Information" (Fig. 1.23).

- Figure 1.23 shows how the time step dynamically changed during the simulation. The algorithm used to dynamically adjust the time step based on the number of iterations needed to solve the Richards equation at any particular time step is described in Chapter 7.4.2 of the Technical Manual. Note that after about 0.65 days, the time step increases significantly. This reflects the fact that the solution is then found much easier (less nonlinear) since the profile approaches steady-state, and HYDRUS-1D hence can use larger time steps.
- Similarly, Figure 1.24 shows that after about 0.67 days, the number of iterations required to achieve a solution drops to the minimum allowed number of 2. Note that very large spikes in the number of iterations may indicate numerical instability, thus warranting a thorough check of the solution integrity (e.g., check mass balance errors).

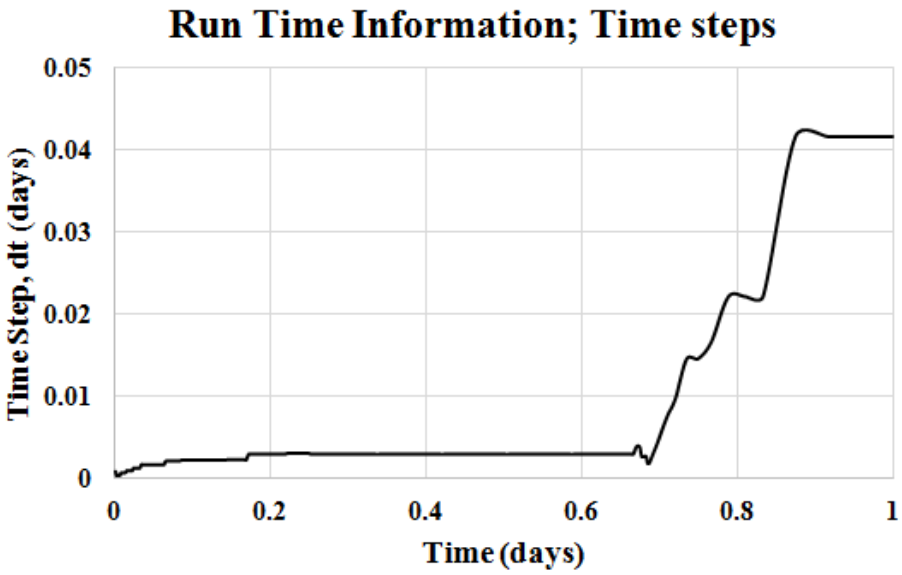

Figure 1.23. Time steps versus time.

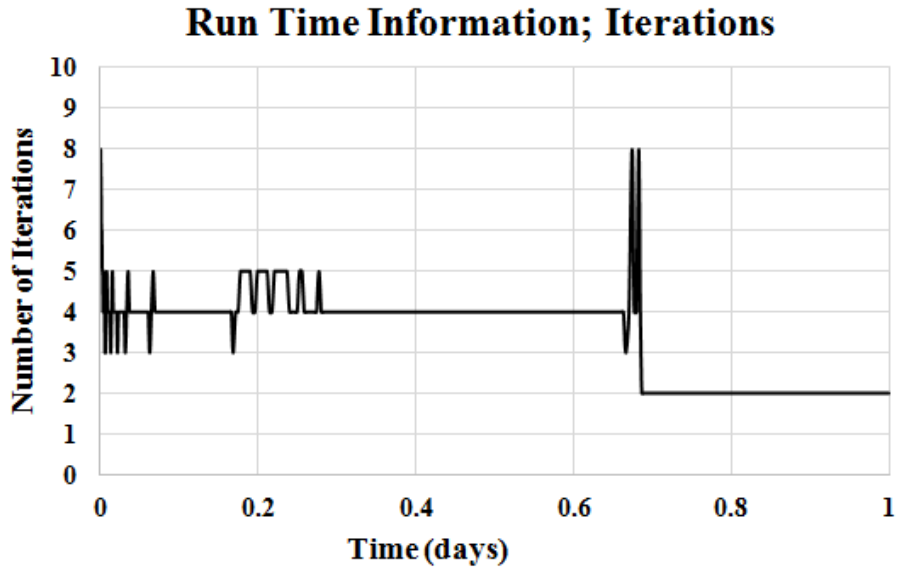

Figure 1.24. The number of iterations versus time.

Mass Balance Information

The output file Balance.out containing the mass balance information at selected print times is displayed under the command "**Mass Balance Information**" of the post-processing section of the HYDRUS-1D GUI (or, again, also using the menu command "Results->Mass Balance Information").

Mass balance information is provided for the entire soil profile and each selected "Subregion" at every "Print Time." Since there is only one subregion in this example, the data in columns 3 and 4 are identical.

Column 1 refers to the following:

Length:	The depth of the soil profile
W-volume:	The total volume of soil water in the soil profile or selected subregions
In-flow:	The sum of fluxes flowing into and out of the soil profile (or subregion)
h Mean:	The average pressure head along the soil profile (or subregion)
Top Flux:	The flux into (at the top) the soil profile
Bot Flux:	The flux out of (at the bottom) the soil profile
WatBalT:	The total (absolute) water balance error for the entire soil profile
WatBalR:	The relative water balance error in % (see Chapter 7.44)

Column 2 gives the units for each variable. The units used are displayed at the beginning of the Balance.out file. In this particular example, L is in cm and T in days.

- Table 1.1 shows that at times up to 0.667 days, the flux into the soil profile is much larger than out of the soil profile.
- Consequently, "In-flow" is positive, which means that water is being stored in the soil profile.
- Table 1.2 shows that at 0.75 days, "In-flow" is zero, thus indicating that a steady-state has been attained (inflow is equal to outflow). This statement is confirmed by the fact that "h Mean" is 1 cm (equal to the imposed upper boundary condition), and the profile is fully saturated (W-volume = Qs x Length = 0.43 x 100 cm = 43 cm). Furthermore, all of the mass balance information for T > 0.75 is identical.

Table 1.1. Mass balance information at Time=0.6667 days.

Time (T)		0.6667	
Sub-region number			1
Length	[L]	1.00E+02	1.00E+02
W-volume	[L]	4.27E+01	4.27E+01
In-flow	[L/T]	2.43E+01	2.43E+01
h Mean	[L]	-9.23E-01	-9.23E-01
Top Flux	[L/T]	-2.53E+01	
Bot Flux	[L/T]	-4.95E+00	
WatBalT	[L]	1.91E-05	
WatBalR	[%]	0.00	

Table 1.2. Mass balance information at Time=0.75 days.

Time (T)		0.75	
Sub-region number			1
Length	[L]	1.00E+02	1.00E+02
W-volume	[L]	4.30E+01	4.30E+01
In-flow	[L/T]	0.00E+00	0.00E+00
h Mean	[L]	1.00E+00	1.00E+00
Top Flux	[L/T]	-2.496E+01	
Bot Flux	[L/T]	-2.496E+01	
WatBalT	[L]	2.86E-05	
WatBalR	[%]	0.00	

Example 2: Infiltration of Water into a Two-Layered Soil Profile

Example Description and Objectives

The objective of this example is to simulate water flow in a 1-m deep, two-layered soil profile. The example demonstrates how to specify time-variable atmospheric boundary conditions (daily values of precipitation and evaporation) and how to interpret simulated results, such as actual boundary fluxes. The soil profile consists of a 50-cm soil layer of clay loam underlain by a 50-cm soil layer of sandy loam. The initially unsaturated soil profile (having a default initial pressure head = -100 cm) is wetted via precipitation during the first 7 days of the simulation. Precipitation changes from 6 cm/d during the first 2 days, to 10 cm/d during the next three days, and finally to 2 cm/d during the last 2 days of the first week. The 'Atmospheric Boundary Condition with a Surface Layer' is invoked, which allows accumulation or ponding of water on the soil surface, with surface runoff occurring only if a user-defined threshold (the maximum ponding depth) has been exceeded. In this example, a different lower boundary condition is imposed, i.e., a 'Seepage Face' boundary condition. Water starts draining from the soil profile through the bottom ' Seepage Face' boundary condition only once the bottom of the profile reaches full saturation (the pressure head becomes zero). As the simulations will show, the soil profile continues to drain until day 10, after which evaporation (1 cm/d) is activated until the end of the 20-day simulation. Note that this is a hypothetical example; neglecting evaporation on certain days allows us to focus on one process at a time (e.g., rainfall, ponding, evaporation).

This example demonstrates the advancement of the wetting front through the two-layered soil profile, calculates prevailing fluxes, and examines the mass balance of each of the two soil layers. The relevance of the pressure head at the seepage face is highlighted. The concept of surface ponding due to a potential flux that exceeds the saturated hydraulic conductivity of the surface soil layer is demonstrated. A suitable Hydraulic Property Model is chosen to cope with the ponding process.

Pre-Processing

Please create 'Example 2' by copying and modifying 'Example 1' using the Project Manager.

Project Manager

- Select *Projects* Tab
- Select *Example 1*
- Click *Button* "Copy"
- Type New Name: Example 2
- Type Description: Infiltration of water into a 2-layer soil profile
- Click *Button* "OK"
- Select *Example 2*
- Click *Button* "Open"

Main Processes

- Heading: Infiltration of water into a 2-layer soil profile

- Click *Button* “Next”

Geometry Information

- Number of Soil Materials: 2 (indicates a two-layered soil profile)
- Number of Layers for Mass Balance: 2 (mass balances will be calculated for each soil layer)
- Click *Button* “Next”

Time Information

Time Discretization:

- Final Time (day): 20
- Maximum Time Step (day): 0.1 (We do not recommend to use a large time step when a surface water layer is allowed to develop (i.e., for saturated near-surface conditions). A larger maximum time step may lead to overshoot in the maximum allowed water layer depth.)
- Check Time-Variable Boundary Conditions (this allows you to specify time-variable precipitation and evaporation fluxes)
- Number of Time-Variable Boundary Records: 5
- Click *Button* “Next”

Print Information

- Number of Print Times: 6
- *Button* “Select Print Times”
- Print Times: 2, 4, 5, 6, 10, 20 days
- Click *Button* “OK”
- Click *Button* “Next”

Water Flow – Iteration Criteria

- Leave default values
- Click *Button* “Next”

Water Flow – Soil Hydraulic Model

- Select the *van Genuchten - Mualem* model *With Air-Entry Value of -2cm* (this model is recommended for very fine textured materials, such as silt loam or clayey soils, or for soils having a van Genuchten *n* parameter smaller than about 1.2; please refer to Appendix III.1.2 and III.2).
- Click *Button* “Next”

Water Flow – Soil Hydraulic Parameters

- Click on the first row: *Mat 1*
- Select from the Soil Catalogue: Clay Loam
- Click on the second row: *Mat 2*
- Select from the Soil Catalogue: Sandy Loam
- Click *Button* “Next”

Water Flow – Boundary Conditions

- Upper Boundary Condition: Atmospheric BC with Surface Layer.
  This boundary condition requires you later to specify time-variable surface fluxes (e.g., rainfall and evaporation rates), while allowing a surface water layer

to build up on the soil surface when some of the rainfall water cannot infiltrate into the soil profile, before surface runoff starts (see Appendix II.1.5).

- Lower Boundary Condition: Seepage Face; **h**=0
  This boundary condition allows water to drain from the soil profile once the pressure head at the bottom of the soil profile reaches a value of 0 (i.e., when full saturation is reached) (see Appendix II.1.7).
- Initial Condition: In Pressure Heads
- Max *h* at Soil Surface: 3 cm
  Surface runoff starts only once the depth of the surface water layer reaches 3 cm.
- Click *Button* "Next"

Time Variable Boundary Conditions

- Fill out the table in the Time-Variable Boundary Conditions dialog window as shown in Figure 2.1.
- The **Precip.** Column. This column indicates that the rainfall rate is 6 cm/d during the first two days (between time 0 and 2 d), 10 cm/d during the next 3 days (between time 2 and 5 d), 2 cm/d during the following 2 days (between 5 and 7 d), and no rainfall during the remainder of the simulation (between times 7 and 20 d). If precipitation data are available from a weather station, then they need to be converted into rates with units corresponding to those used in HYDRUS-1D as defined during geometry and time information preprocessing (more details can be found in Appendix II.1.5.
- The **Evap.** column. This column indicates that there is no evaporation during the first 10 days and evaporation of 1 cm/d between day 10 and 20. We assume that evaporation is negligible during (first seven days) and immediately after (next three days) the rainfall event.
- The **hCritA** column. This parameter indicates that actual evaporation remains equal to potential evaporation until the pressure head in the top node reaches -50,000 cm. Once the **hCritA** value is reached, the actual evaporation rate becomes lower than the potential value since the soil is then too dry to deliver the potential rate. The **hCritA** parameter (given here in absolute values) is not used in any other calculation, except for evaluating evaporation rates. Note that you can click on the corner of a cell and copy values downward by dragging the cursor, similarly as in an Excel spreadsheet; in this case, you can do this for the hCritA column]
- Click *Button* "Next"

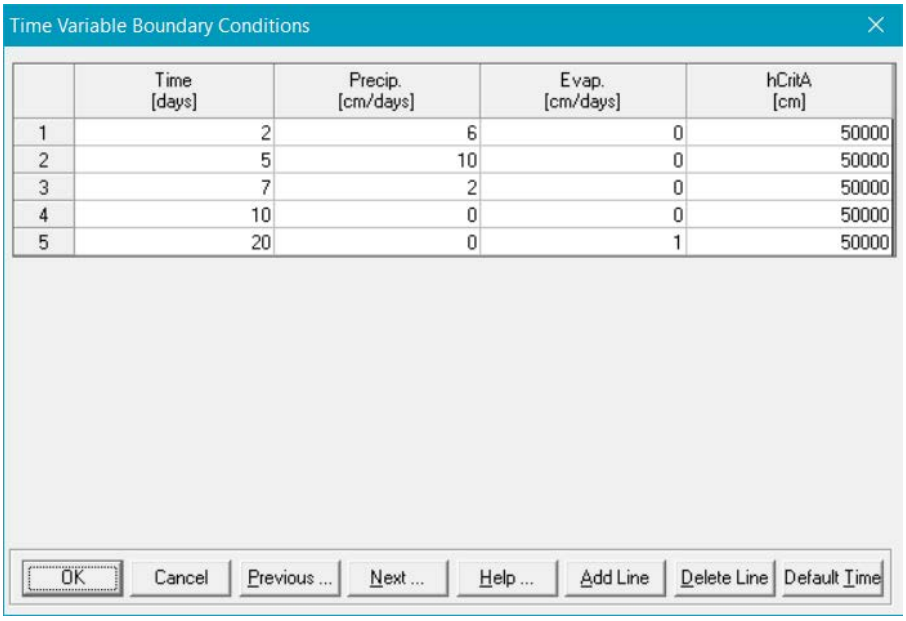

Figure 2.1. The **Time-Variable Boundary Conditions** dialog window.

HYDRUS-1D Guide

- Do you want to run PROFILE application?
- Click *Button* "OK"

Soil Profile – Graphical Editor

The **Soil Profile** editor allows you to specify the initial pressure head condition, the distribution of soil materials and soil layers versus depth for mass balance calculations, and the location of observation nodes.

- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar**
- Click the "Edit Condition" *Button* on the left-side Edit Bar, select with the Mouse the entire soil profile, left click the mouse again, and specify a pressure head of -100 cm.
  (The entire profile will be at the default initial pressure head of -100 cm)
- **Menu**: Conditions->Material Distribution or **Toolbar**
- Click the "Edit Condition" *Button* on the left-side Edit Bar, select with the Mouse node 52 to 101 (left click at node 52, drag the mouse to the bottom node, and left click again).
- In the "Condition Specification" dialog window, set the **Material Index** equal to 2 and click OK (Material 2 corresponds to the second layer, the sandy loam; Material Index 1 corresponds to the clay loam layer).
- **Menu**: Conditions->Subregions or **Toolbar**
- Repeat the same process (as for Material Distribution); set the **Subregion Index** equal to 2 for nodes between 52 and 101 and click OK. In this way the Mass Balance will be calculated separately for Material 1 and 2, together with the Mass Balance for the entire profile.
- **Menu**: Conditions->Observation Nodes or **Toolbar**
- Click the "Insert" *Button* on the left-side Edit Bar and select nodes at 0, 50, and 100 cm (right-click to end the command)
- **Menu**: File->Save Data or **Toolbar**

- **Menu**: File->Exit

Soil Profile – Summary

- Click *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or use the **Toolbar** button  .

Post-Processing

Observation Points

Referring to Figure 2.2:

- Note that the pressure head at the surface node (ON-1 at 0 cm) becomes positive after two days when the precipitation rate of 10 cm/day exceeds the saturated hydraulic conductivity of the upper Clay Loam layer (6.24 cm/day). The pressure head (reflecting the thickness of the surface water layer) continues to increase up to the preset limit of 3 cm, at which time surface runoff is triggered (day three). At this stage, the boundary condition switches to a "Constant Head" boundary condition and surface runoff is calculated subsequently as the difference between the precipitation and infiltration rates (both instantaneous and cumulative runoff is stored as output and can be displayed upon request). Note that during the first time step when the maximum thickness of the water layer is reached, the pressure head may slightly rise above 3 cm. HYDRUS-1D will then force it back to the prescribed 3 cm during the next time step. This breach can be limited by setting a smaller "Maximum Time Step" (say, 0.01 day).
- For times between day 3 and day 5, the profile has attained a steady-state condition (all three pressure heads are constant; horizontal lines).
- When the precipitation rate drops below the saturated hydraulic conductivity of the surface layer (clay loam, 6.24 cm/day) at day 5, all of the precipitation stored in the surface water layer gradually infiltrates into the soil profile and the soil surface becomes unsaturated again (at about 5.5 d).
- After the cessation of precipitation (Time > 7 d) and before the activation of evaporation (at day 11), the pressure heads in the soil profile continue to decrease as a result of drainage due to gravity. During this period, the lower boundary (ON-3 at 100 cm) remains saturated, and water continues draining out of the bottom of the soil profile through the seepage face.
- At day 11, evaporation is activated, and hence the soil profile starts drying out at a much faster rate. The pressure head at the soil surface eventually reaches the minimum allowed pressure head 'hCritA' of -50,000 cm (not shown in Figure 2.2). The drying process progresses down through the soil profile until it reaches the lower Seepage Face boundary at about 13.4 days. Then, the bottom boundary becomes unsaturated, and hence the seepage flux ceases.

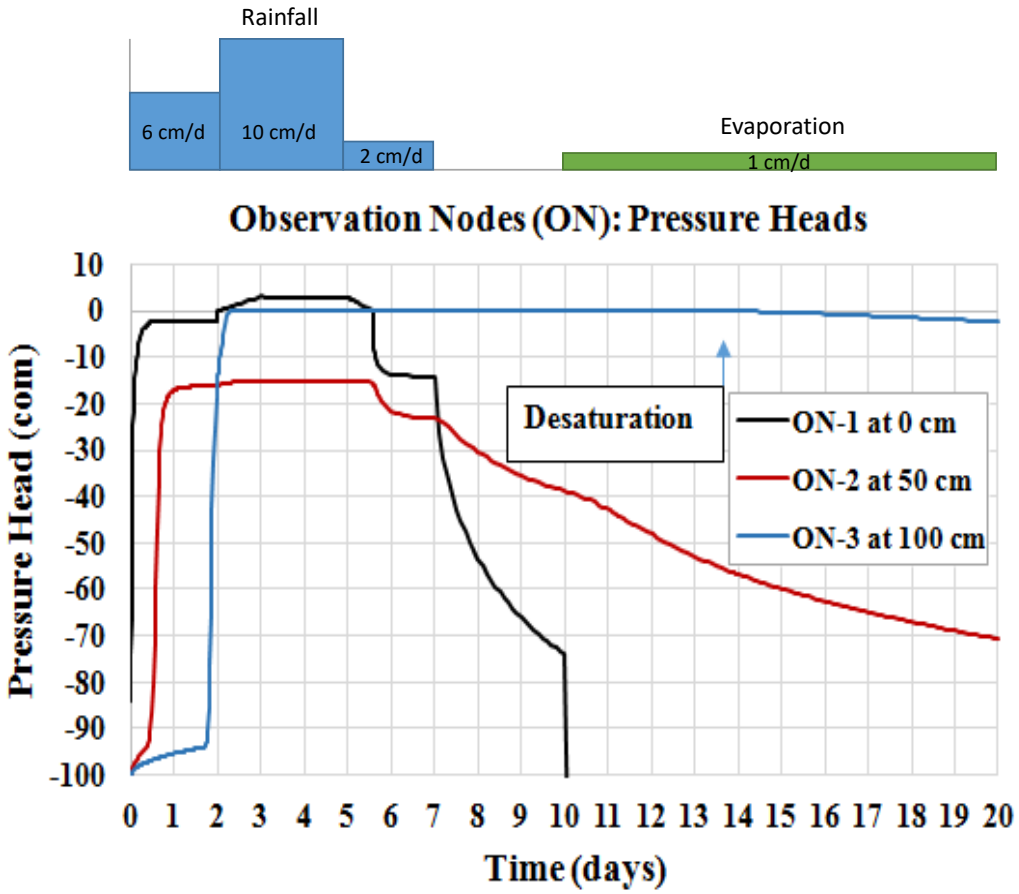

Figure 2.2. Pressure heads versus time at selected observation points. The upper part of the figure shows the applied boundary conditions.

Profile Information

Referring to Figure 2.3:

- The pressure head profile at day 2 indicates that the lower boundary has not yet reached full saturation (pressure head < 0), which means that there is no bottom flux.
- The pressure head profiles at days 4 and 5 are identical, which confirms that a steady- state has indeed been attained during this period.
- On the other hand, the bottom pressure head is equal to zero from day 4 to day 10, indicating draining of the soil profile through the bottom boundary.

Referring to Figure 2.4:

- Note the abrupt change in the water content at the interface between the two soil types. While the pressure head across the material interface is continuous (Figure 2.3), the water content is not so due to the different water retention properties (and thus retention curves) of the two materials. Also note that while the pressure head across the material interface is continuous, its gradient above and below the interface is discontinuous due to different conductivities of the two materials. The pressure head gradients at the material interface need to compensate the different hydraulic conductivities of the two materials since the water flux is the same when approaching the interface from above and below.

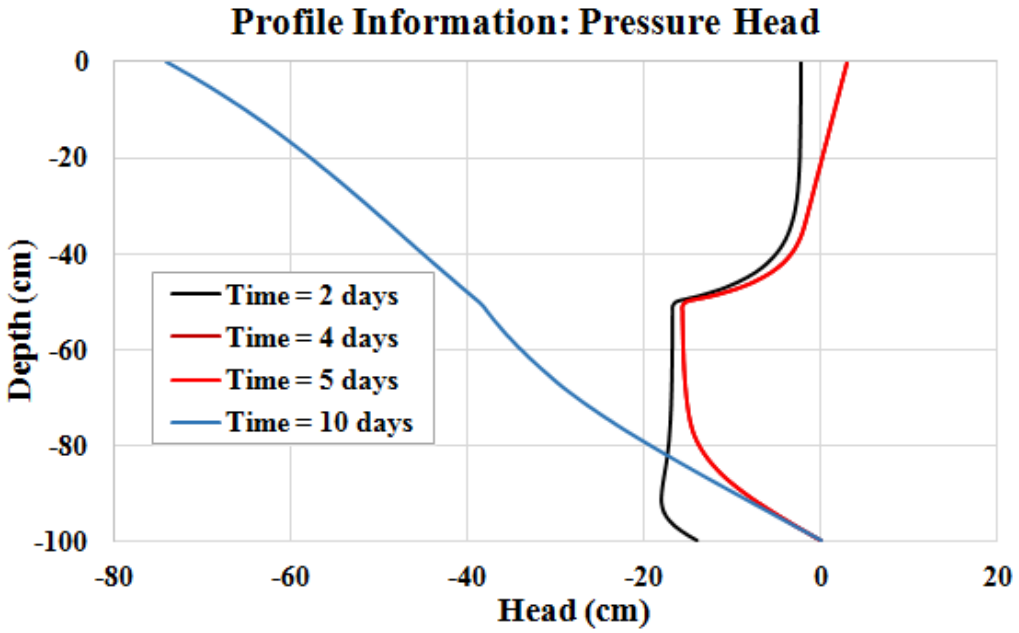

Figure 2.3. Pressure head profiles at selected times. The boundary between layer 1 (clay loam) and layer 2 (sandy loam) is at -50 cm.

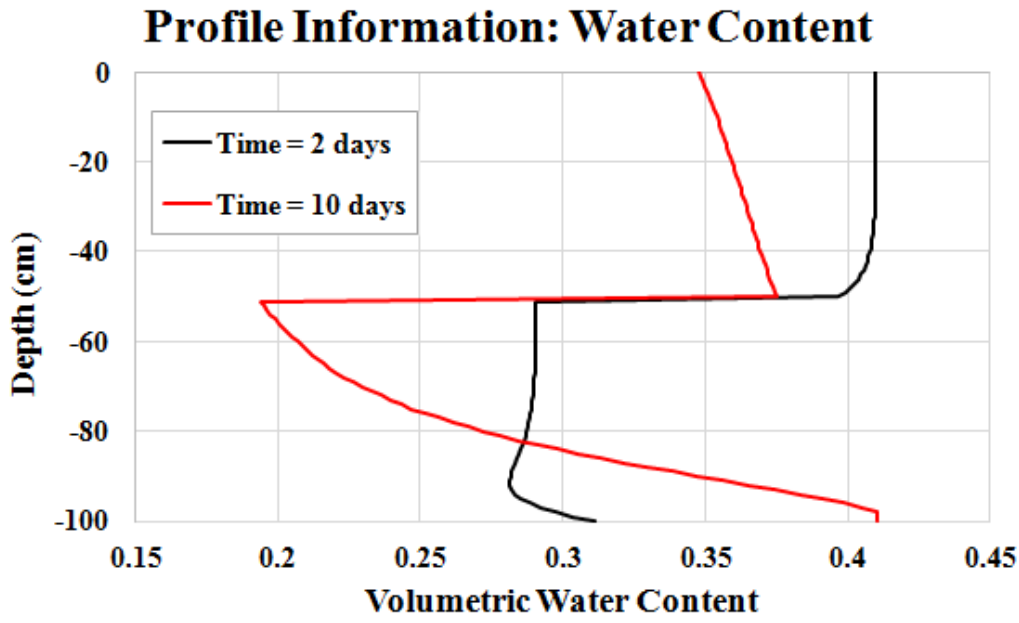

Figure 2.4. Water content profiles at selected times. The boundary between layer 1 (clay loam) and layer 2 (sandy loam) is at -50 cm.

Water Flow - Boundary Fluxes and Heads

Referring to Figure 2.5:

- Note that HYDRUS-1D reports downward fluxes (against the upward direction of the *z*-axis) as negative and upward fluxes (in the direction of the *z*-axis) as positive.
- The surface flux between days 0 and 2 is equal to the applied precipitation rate of 6 cm/day since this rate is lower than the saturated hydraulic conductivity of the surface soil layer (clay loam, 6.24 cm/day).
- Once the precipitation rate is higher than the saturated hydraulic conductivity of the surface soil layer, the soil surface quickly reaches full saturation, and excess water (the difference between the rainfall and the infiltration rates) starts to accumulate at the soil surface.
- Before the surface becomes fully saturated (at time > 2 d), the infiltration rate can be higher than the saturated hydraulic conductivity of the surface layer because of the capillary component of the total gradient.
- Once full saturation is reached, and the surface water layer gradually increases until it reaches its maximum thickness of 3 cm (between 2 and 3 d), the infiltration rate gradually increases as well because of the additional contribution to the total gradient by the hydrostatic pressure due to the surface water layer.
- The infiltration flux stabilizes once the maximum thickness of the surface water layer (3 cm) is reached.
- Between 4 and 5 days, the flux into the soil profile is equal to the flux out of the soil profile, which confirms that the soil profile has attained a steady-state.
- The infiltration rate starts decreasing when the precipitation rate becomes smaller than the saturated hydraulic conductivity (K_s) but remains approximately equal to K_s as water from the surface layer infiltrates.
- As soon as the bottom of the profile becomes saturated (between day 2-3), drainage commences. Water continues flowing through the lower 'Seepage Face' boundary as the profile continues to drain due to gravity.
- The seepage flux ceases at 13.4 days when the pressure head at the lower boundary becomes negative (desaturation).
- The actual surface evaporative flux (positive) is equal to the applied potential evaporation rate of 1 cm/day up to about 11.2 days (as long as the surface pressure head is higher than hCritA), after which it drops as the soil surface dries out and the hydraulic conductivity can no longer sustain this evaporative flux.

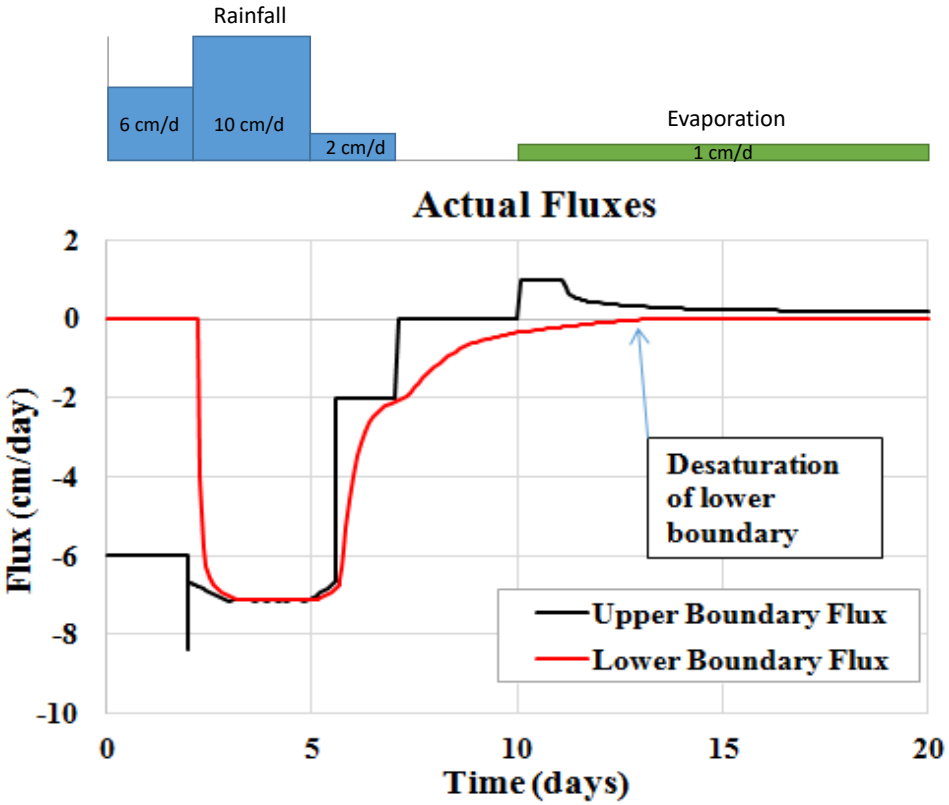

Figure 2.5. The surface (into the soil profile) and bottom (out of the soil profile) fluxes versus time. The upper part of the figure shows the applied boundary conditions.

Mass Balance Information

- Table 2.1 shows the mass balance information for the layered soil profile. Note that, in addition to the mass balance for the entire profile (the first data column), a separate mass balance is provided for the two subregions: the top 50 cm (the second data column) and the bottom 50 cm (the third data column).

Table 2.1. The mass balance information for Time = 10 days.

Time	day	10		
Sub-region	number		1	2
Length	cm	100	50	50
W-volume	cm	31.8	18.1	13.7
In-flow	cm/day	-0.348	-0.194	-0.154
h Mean	cm	-38.6	-55.1	-22.2
Top Flux	cm/day	-0.00225		
Bot Flux	cm/day	-0.348		
WatBalT	cm	-1.62E-05		
WatBalR	[%]	0.00		

Example 3: Root Water Uptake

Example Description and Objectives

The objective of this example is to simulate water flow and root water uptake in a 3-m deep uniform soil profile and to demonstrate how to simulate root water uptake and associated crop transpiration processes. The soil profile is initially at hydrostatic equilibrium, i.e., the pressure head changes uniformly from -300 cm at the top of the soil profile to 0 cm at the bottom. The profile is wetted via precipitation through an 'Atmospheric Boundary with Surface Runoff' during the first three days, while evaporation and transpiration (Evapotranspiration, ET) are active during the entire 30-day simulation. The bottom boundary is a 'Constant Head Boundary', with a 0-cm constant pressure head representing the groundwater table. Roots are uniformly distributed from the surface down to a depth of 200 cm, which is still 100 cm above the groundwater table.

This example simulates root water uptake and its reduction due to the water stress when the soil can no longer supply water to the plant roots at an optimal rate. Project results will show how pressure heads and water fluxes evolve differently at various depths in the soil profile as a result of the combined processes of infiltration, evaporation, and transpiration. The default (uniform) spatial discretization is changed so as to demonstrate how to specify a finer grid at some locations. The phenomenon of 'groundwater ET', whereby the plant sources its water by capillary action from the underlying groundwater aquifer (despite the fact that roots are well above the water table), is demonstrated using this example.

Pre-Processing

Project Manager

- Open the **Project Manager** (from the File Menu or the third button on the Toolbar, ).
- Select *Projects* Tab
- Click button "New"
- Type the **Name** of the project: "Example 3"
- Type the **Description** of the project: Root water uptake in a soil profile
- Click *Button* "OK"

Main Processes

- Heading: Root water uptake in a soil profile
- Check the *Root Water Uptake* checkbox (in addition to already checked Water Flow)
- Click *Button* "Next"

Geometry Information

- Length Units: cm
- Number of Soil Materials: 1 (indicates a homogenous soil profile)
- Number of Layers for Mass Balance: 1 (one may select up to 10 mass balance layers)
- Decline from vertical axis: 1 (vertical flow)

- Depth of Soil Profile (cm): 300 cm
- Click *Button* “Next”

Time Information

- Time Units: Days
  Time Discretization:
- Initial Time (day): 0
- Final Time (day): 30
- Initial Time Step (day): 0.001
- Minimum Time Step (day): 0.00001
- Maximum Time Step (day): 5
- Check Time-Variable Boundary Conditions
- Number of Time-Variable Records 2
- Click *Button* “Next”

Print Information

- Print Options: Leave as Default
- Number of Print Times: 11
- Click *Button* “Select Print Times”
- Print Times (day): 1, 2, 3, 4, 5, 6, 7, 8, 10, 15, 30
- Click *Button* “OK”
- Click *Button* “Next”

Water Flow – Iteration Criteria

- Leave default values
- Click *Button* “Next”

Water Flow – Soil Hydraulic Model

- Check the Single Porosity model: van Genuchten – Mualem
- Check "With an Air-Entry Value of -2 cm" (this model is recommended for fine textured materials, such as clayey soils, or for soils with the *n* parameter smaller than about 1.2)
- Click *Button* “Next”

Water Flow – Soil Hydraulic Parameters

- Select Clay from the Soil Catalogue
- Click *Button* “Next”

Water Flow – Boundary Conditions

- Upper Boundary Condition: Atmospheric BC with Surface Run Off
  (surface runoff is initiated immediately once the precipitation rate exceed the infiltration rate. At the same time, the flux boundary condition is replaced with the pressure head boundary condition with zero pressure head. Under this boundary, condition excess precipitation does not accumulate at the surface).
- Lower Boundary Condition: Constant Pressure Head
  (this boundary condition with a zero pressure head will indicate that the groundwater level is at the bottom of the soil profile and is constant in time).
- Initial Condition: In Pressure Heads
- Click *Button* “Next”

Root Water and Solute Uptake Model

In the **Root Water and Solute Uptake Model** dialog window (Fig. 3.1.) you can select which model to use to account for the effects of **water stress** on root water uptake, either the *Feddes* (1977) model or an *S-shape* function (van Genuchten, 1987) can be used, and whether or not (*No Solute Stress*) should be considered to account for **salinity stress**. Salinity stress can be either additive (*Additive Model*) or multiplicative (*Multiplicative Model*), and either the threshold and slope model (Maas, 1990) (*Threshold Model*) or the S-shaped (*S-Shape*) function (van Genuchten, 1987) can be used. It is also possible to consider either non-compensated (the *Critical Stress Index* = 1) or compensated (the Critical Stress Index < 1) root water uptake. You can additionally consider **Active Solute Uptake** (Šimůnek and Hopmans, 2009) and specify related parameters. Root water and solute uptake are described in detail in Chapter 2.2 and 3.5, respectively, of the Technical Manual.

Root Water Uptake Reduction Model
- Check Feddes (Default)
- Click *Button* "Next"

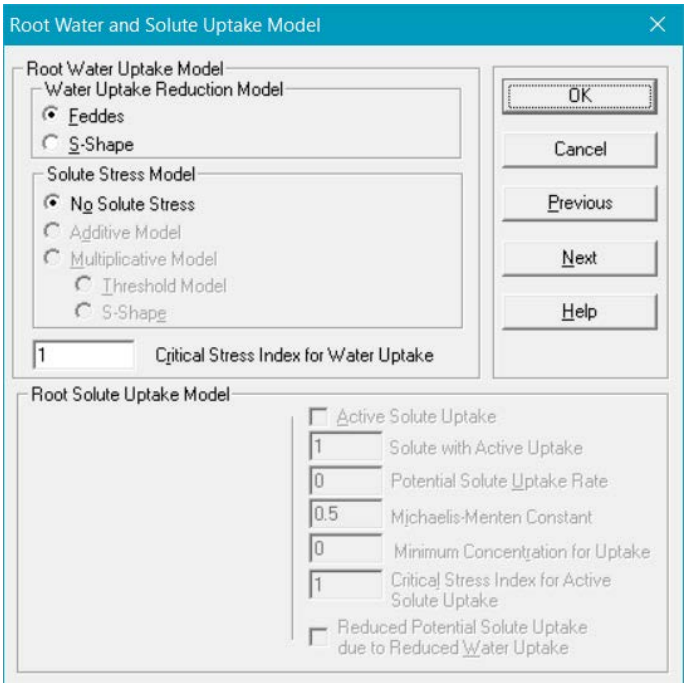

Figure 3.1. The **Root Water and Solute Uptake Model** dialog window.

Root Water Uptake Parameters

Parameters for the water stress response functions are specified in the **Root Water Uptake Parameters** dialog window (Fig. 3.2). The **Root Water Uptake Parameters** for the water stress response function suggested by Feddes et al. **(**1978) are described in detail in the HYDRUS-1D technical manual. Water uptake in this model is assumed to be zero close to saturation (i.e., wetter than some arbitrary "anaerobiosis point" **P0**). Root water uptake is also zero for pressure heads less (more negative) than the wilting point (**P3**). Water uptake is considered optimal between pressure heads **Popt** and **P2**, whereas for pressure heads between **P2** and **P3** (or **P0** and **Popt**) water uptake decreases

(or increases) linearly with pressure head. Root water uptake occurs at its optimal value even at full saturation, when both P0 and POpt are set equal to zero.

- Select *Pasture* (default) from the Database (all parameters will then be populated automatically with values from the implemented database)
- Click *Button* "Next"

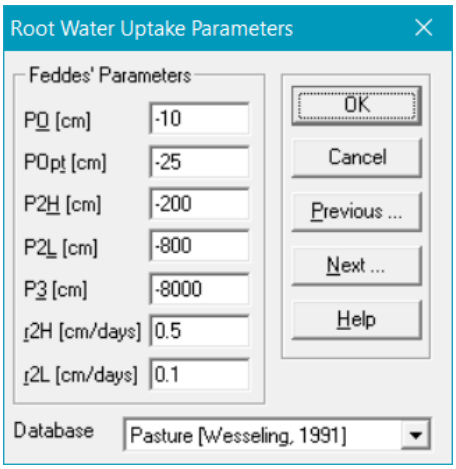

Figure 3.2. The **Root Water Uptake Parameters** dialog window.

Time Variable Boundary Conditions

In this dialog window, specify a rainfall rate of 2 cm/d during the first two days, an evaporation rate of 0.1 cm/d during all 30 days of simulation, and a transpiration rate of 0.5 cm/d during the first 3 and 1.5 cm/d during the subsequent 27 days.

- Row 1: Time=3 day; Precip=2 cm/day; Evap=0.1 cm/day; hCritA=50,000 cm; Transp=0.5 cm/day
- Row 2: Time=30 day; Precip=0 cm/day; Evap=0.1 cm/day; hCricA=50,000 cm; Transp=1.5 cm/day
- Click *Button* "Next"

HYDRUS-1D Guide

- Do you want to run PROFILE application?
- Click *Button* "OK"

Soil Profile – Graphical Editor

You can use the **Soil Profile** editor to adjust the spatial discretization of the soil profile (in this case smaller elements at the top and bottom boundaries, with the element size increasing by a geometric factor from both top and bottom towards the middle of the profile), specify the initial pressure head conditions, the root distribution with depth, and the position of observation nodes.

- **Menu**: Conditions->Profile Discretization or **Toolbar** 
- Click the "Number" button on the left-side Edit Bar: Number of Nodes = 120.
- Click the "Insert Fixed" button: Select the Node at a depth of 150 cm (the midpoint of the profile). These points are used to specify the local nodal density.

By default, they are placed at the upper and lower boundaries, but in addition can be inserted at, or deleted from, any other point in the soil profile.
(Note that when you move the cursor around the view window, you can monitor its position, i.e., the node numbers and the depth, at the lower right corner)

- Click the "Density" button, select the top node, left click the mouse button, in the **Nodal Density** dialog window enter the *Lower Density* of 0.1, and click the OK button.
- Click the "Density" button again, select the bottom node, left click the mouse button, in the **Nodal Density** dialog window enter the *Upper Density* of 0.3, and click the OK button.
  Note that the FE nodes will get automatically redistributed proportionally based on the specified densities. The distance between nodes at the top will be (1/0.1=) 10 times smaller than in the middle, while the distance between nodes at the bottom will be (1/0.3=) 3.33 times smaller than in the middle. The nodal density is a real number between 0.01 and 100, specifying the local density of nodes. The density can be specified only at fixed points (either at the top or bottom boundary or at an additional user-defined "Insert Fixed" node). The program distinguishes between top and bottom density. At the top (bottom) boundary, only the Lower Density (Upper Density) can be specified. For any inserted fixed node, the top (bottom) density at a fixed point specifies the relative thickness of the elements above (or below) this point. If the top and bottom densities are equal, then the elements above and below the fixed node will have the same thickness. If the top and bottom density values are different, then the element thicknesses will be different as well.
- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar** 
- Click the "Edit Condition" button (left side), select with the Mouse the entire profile, left click the mouse button, in the **Condition Specification** dialog window that appears enter *Pressure Head Distribution*: Top value=-300 cm and Bottom value=0 cm, uncheck '*Use top value for both*', and click the OK button.
- **Menu**: Conditions->Root Distribution or **Toolbar** 
- Click the "Edit Condition" button (left side), select with the Mouse the nodes down to a depth of 200 cm, left click the mouse again, in the **Condition Specification** dialog window that appears enter *Roots Linear Distribution*: Top value=1, check 'Use top value for both', and click the OK button. This means that roots are distributed uniformly in the top 200 cm of the soil profile.
  Typical root distribution functions are shown in Figure 3.3. Note that HYDRUS-1D can accommodate any arbitrarily measured or prescribed root distribution function by using the Root Distribution function.
- **Menu**: Conditions->Observation Nodes or **Toolbar** 
- Click the "Insert" *Button* on the left-side Edit Bar and specify nodes at 0 and 300 cm (right-click to end the command)
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

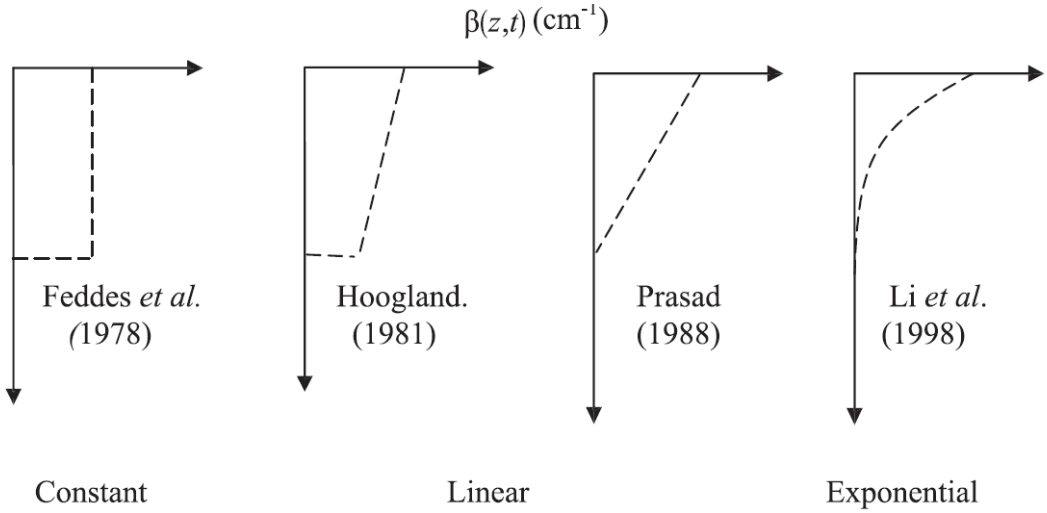

Figure 3.3. Schematic of possible root distribution functions (Kumar et al., 2014).

Soil Profile – Summary

- Click *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D, or a Toolbar button  .

Post-Processing

Observation Points

Referring to Figure 3.4:

- The pressure head in the surface node (ON-1 at 0 cm), which was initially at a pressure head of -300 cm, increases during the first three days of the simulation as a result of precipitation and infiltration. Subsequently, the pressure head decreases down to the minimum limit of hCritA (-50,000 cm) as a result of evaporation (the minimum value shown in Figure 3.4 is -500 cm).
- The pressure head at the bottom node (ON-2 at 300 cm) remains constant at 0 cm (i.e., the Constant Pressure Head boundary condition representing the groundwater table).
- The full pressure head range (-50,000-0 cm) and total simulation time (0-30 d) are not shown in Figure 3.4 in order to highlight the changes at early times.

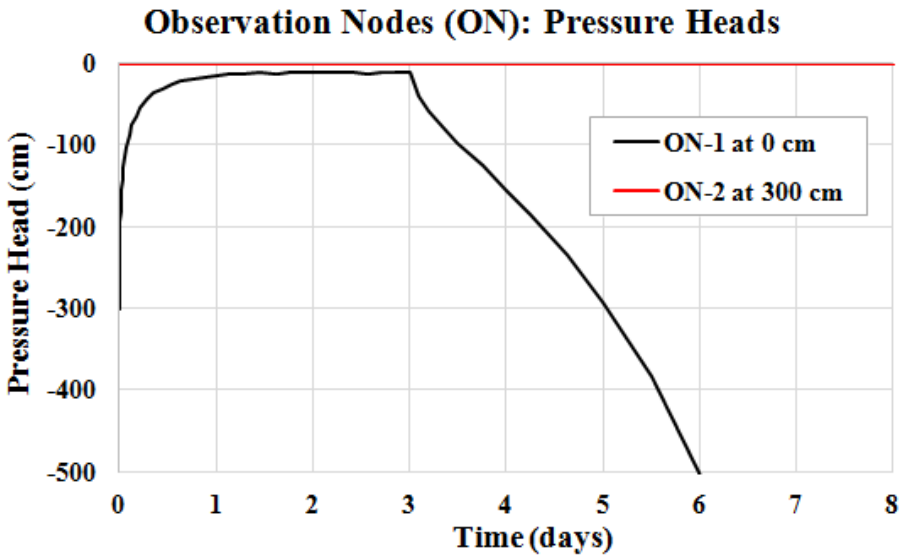

Figure 3.4. Pressure heads versus time at selected observation points.

Profile Information

Referring to Figure 3.5:

- The pressure head profiles at days 1 and 3 show the typical advance of the wetting front during the precipitation period, up to day 3.
- The pressure head at day 6 displays a drying profile due to the combined effects of transpiration and evaporation; drying is most pronounced at the soil surface due to the evaporation boundary. The effect of transpiration on the soil pressure head and water content distributions are depth-dependent and visualized by means of the root water uptake function.

Referring to Figure 3.6:

- As a result of the low transpiration rate (0.5 cm/day), root water uptake at t = 1 day is limited to just above 0.002 day^{-1}; water uptake is maximal from about -25 cm down to the bottom of the roots (-200 cm).
- When transpiration increases at the beginning of day 3 from 0.5 to 1.5 cm/day, root water uptake in the top of the profile is suboptimal owing to the pressure head being greater (i.e., less negative) than the optimal pressure head (Popt = -25 cm; see Figure 3.2).
- At time = 6 and 10 days, root water uptake has tripled following the increase in transpiration. At t = 6 days water uptake is nearly uniform in the entire root zone. As the profile starts drying out at the top (see pressure head evolution in Figure 3.5), water uptake will progressively be from deeper depths.

Referring to Figure 3.7:

- Time = 1 day: Near the surface, the downward (negative) flux reflects infiltration due to precipitation (the surface flux equals evaporation-precipitation: 0.1-2=-1.9 cm/d) with the wetting front approaching a depth of 100 cm. However, below a depth of 130 cm, there is a small positive upward flux from the constant head boundary (the water table) to the soil profile driven by plant uptake. Note the zero-flux point at a depth of about 130 cm.

- Time = 3 days: The wetting front advances deeper into the soil profile and provides plants with its water demand (and hence there is no upward positive flux from the water table at this time). Water infiltrating through the upper "atmospheric" boundary (due to precipitation) drains through the bottom "constant pressure head" boundary.
- Time = 5 days: The upper 70 cm of the profile is drying out due to evaporation. As a result, a net positive upward flux occurs out of the soil profile through the upper "atmospheric" boundary. As the upper part of the profile gets drier, roots start to source their water via an upwards flux from the bottom "constant head" boundary (note the positive flux below a depth of 150 cm).
- Time = 30 days: The top 150 cm of the soil profiles becomes so dry that the upward flux practically ceases and the pressure head at the soil surface reaches the limiting hCritA value (-50,000 cm). Transpiration (root water uptake) also ceases in this part of the profile where the pressure head drops to or below the wilting point (P3) of -8000 cm (note the pressure head distribution in Figure 3.8). It is the high pressure head gradient between the lower part of the root zone (below 130 cm) and the "constant head" boundary that drives the upward flux from the water table to satisfy part of the plant water demand (in this case, roots between depths of 130 cm and 200 cm are sourcing their water demand from groundwater). Note that the fine-textured clay soil has a high air-entry value and a high capacity to maintain the soil close to saturation, thus promoting this phenomenon.

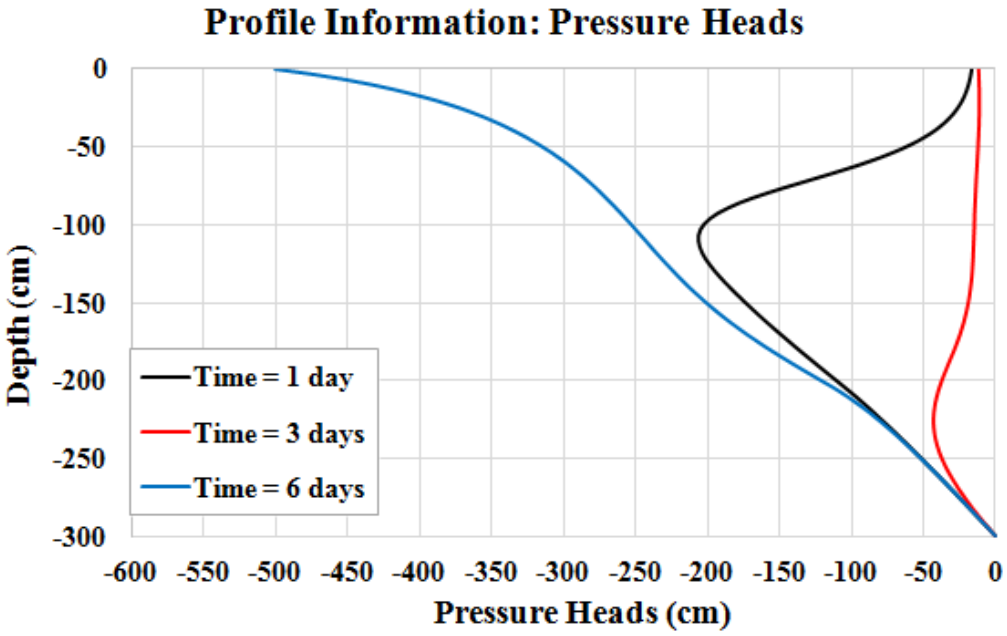

Figure 3.5. Pressure head profiles at selected print times. The bottom boundary condition corresponds to a groundwater table with h = 0 cm.

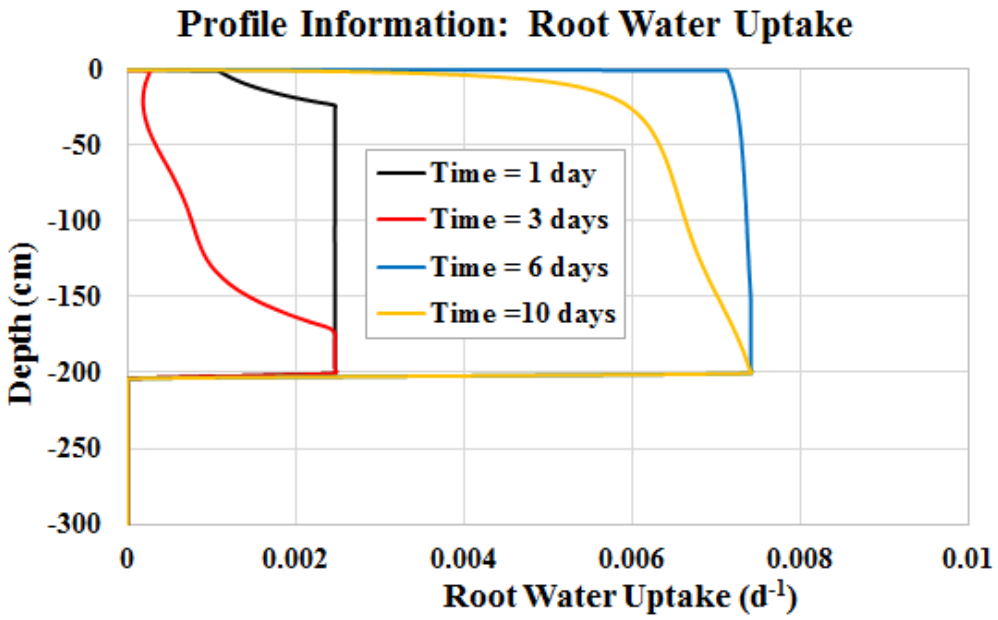

Figure 3.6. Root water uptake at selected print times.

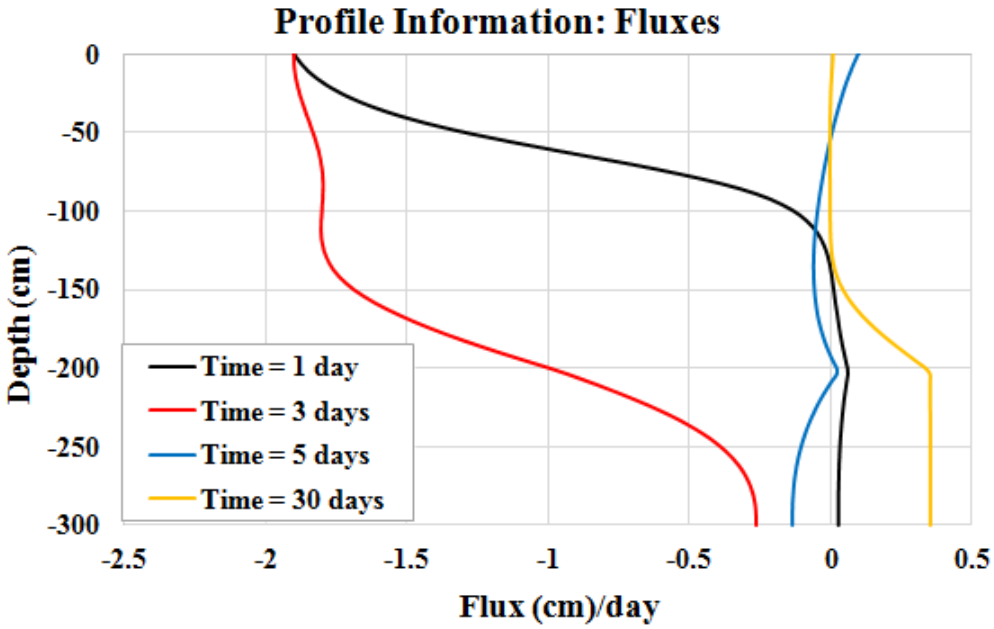

Figure 3.7. Flux profiles at selected print times.

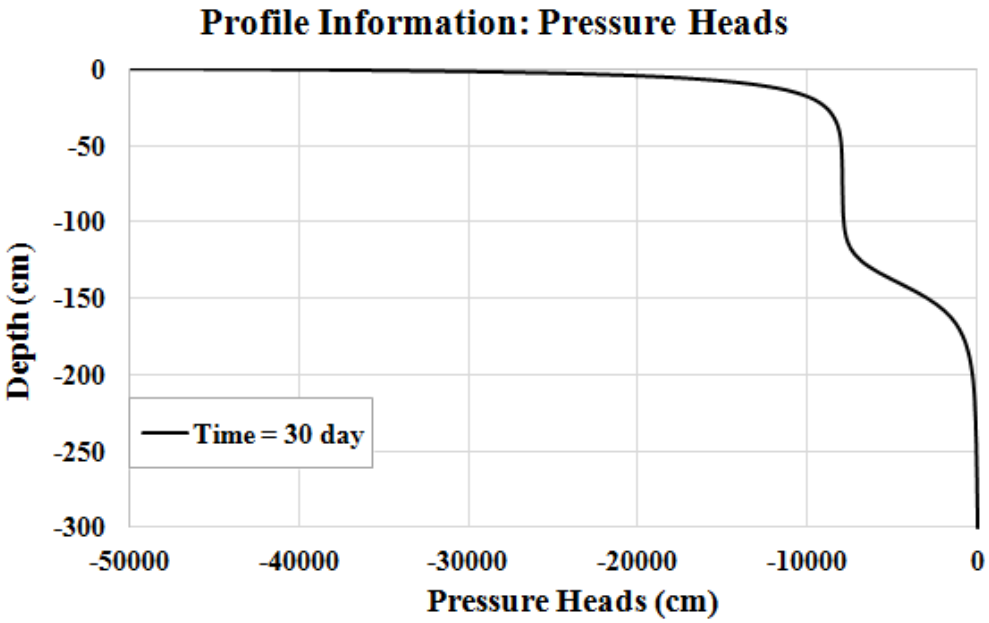

Figure 3.8. Pressure head profile at Time = 30 days.

Water Flow - Boundary Fluxes and Heads

Referring to Figure 3.9:

- The upper boundary flux is equal to precipitation minus evaporation (2 cm/day – 0.1 cm/day) during the first three days. After day 3 when precipitation ceases, the flux becomes positive (the upward flux from the atmospheric boundary) due to evaporation. The actual flux remains equal to the potential flux up to day 12 (the first stage of evaporation), after which it drops below the potential value (the second stage of evaporation), until it becomes very small (about 0.01 cm/day at day 30).
- Actual root water uptake remains equal to potential (0.5 cm/day) for a short period of time, after which it starts to decrease. Potential transpiration increases to 1.5 cm/day after 3 days. Actual transpiration continues to drop until it is approximately equal to the upward flux from the "constant head" bottom boundary. At that time, the soil profile attains a steady-state condition.
- The lower boundary flux is initially zero since the initial condition was equal to the hydrostatic condition. Due to root water uptake drawing water up into the profile, the bottom flux starts gradually increasing (representing an upward flux from the water table). After about two days, the precipitation front reaches the bottom boundary and reverses the bottom flux to be negative. Following the cessation of precipitation, the trend reverses again due to the root water demand. The flux eventually reaches a steady-state, satisfying about 23% of the root water demand (the long-term upward flux = 0.366 cm/day, potential transpiration = 1.5 cm/day).

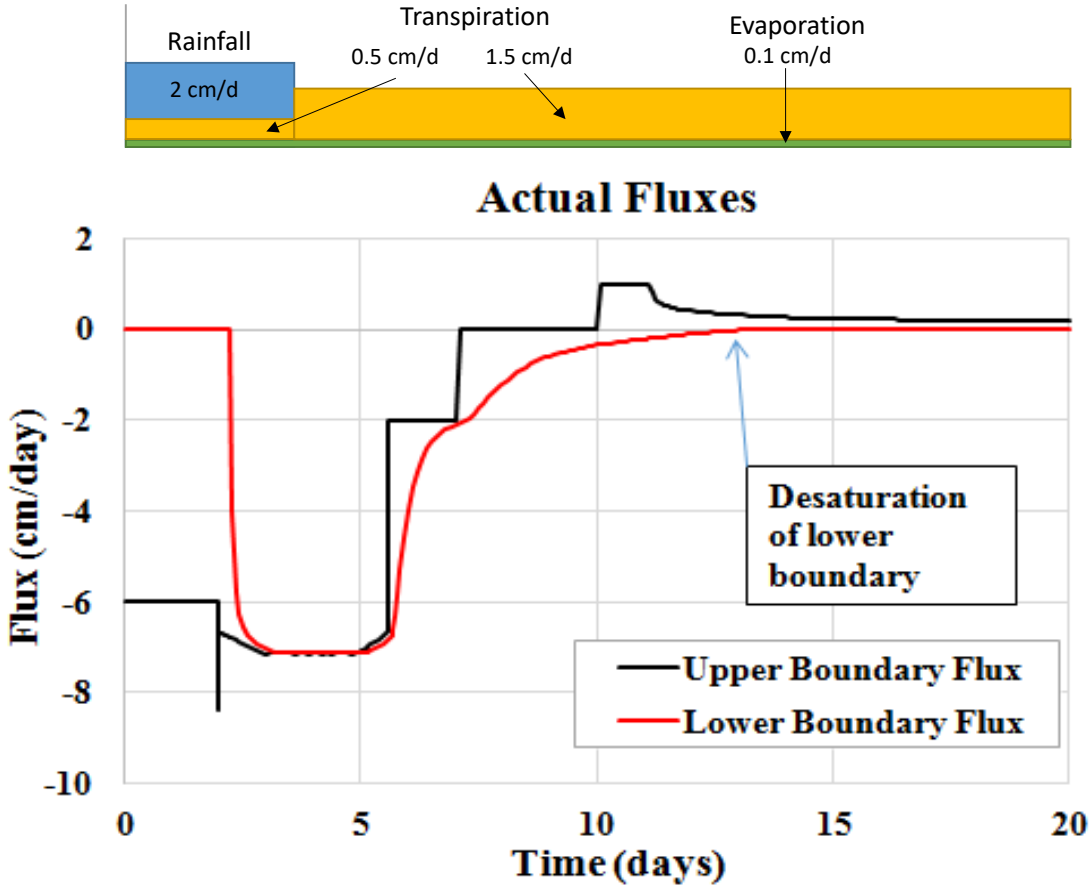

Figure 3.9. The surface flux (into the soil profile), root water uptake (from within the soil profile), and the bottom flux (out of the soil profile) versus time. The upper part of the figure shows the applied boundary conditions.

Example 4: Estimating Groundwater Recharge

Example Description and Objectives

The objective of this example is to simulate water flow and root water uptake in a 100-cm deep uniform soil profile and to evaluate flow across the bottom boundary of the profile (i.e., groundwater recharge). The soil profile is initially at a uniform pressure head equal to -100 cm. The boundary condition for the soil surface is an 'Atmospheric Boundary Condition with Surface Runoff'. The bottom boundary condition is 'Free Drainage' (i.e., the groundwater table is assumed to be deep enough to not influence water redistributions in the soil profile). Roots are uniformly distributed from the soil surface down to a depth of 50 cm. A 366-day time series of meteorological data from the Tully region in north Queensland, Australia, is provided, which allows you to calculate daily values of potential evapotranspiration. The HYDRUS-1D model is thus used to calculate actual plant water uptake (i.e., actual transpiration) and to estimate deep drainage below the root zone, which eventually recharges the underlying aquifer.

Pre-Processing

Project Manager

- Select *Projects* Tab
- Click *Button* "New"
- Type Name: Example 4
- Type Description: Root uptake with meteorological data
- Click *Button* "OK"

Main Processes

- Heading: Root uptake with meteorological data
- Check "Root Water Uptake" (in addition to a default process "Water Flow")
- Click *Button* "Next"

Geometry Information

- Length Units: cm
- Number of Soil Materials: 1 (indicates a homogenous soil profile)
- Number of Layers for Mass Balances: 1 (users may select up to 10 mass balance layers)
- Decline from vertical axis: 1 (vertical flow)
- Depth of Soil Profile (cm): 100 cm
- *Button* "Next"

Time Information

- Time Units: Days
  Time Discretization:
- Initial Time (day): 0
- Final Time (day): 366
- Initial Time Step (day): 0.001
- Minimum Time Step (day): 0.00001
- Maximum Time Step (day): 5
- Check "Time-Variable Boundary Conditions"

- Number of Time-Variable Boundary Records: 366
- Check "Meteorological Data"
- Number of Meteorological Records: 366
- Select "Penman-Monteith Equation" (Default)
- *Button* “Next”

Note that contrary to previous examples with **Time-Variable Boundary Conditions** when users specify directly the potential transpiration and evaporation rates, in this example these rates (or a combined evapotranspiration rate) will be evaluated from **Meteorological Data** (e.g., solar radiation, wind speed, air temperature and humidity) using the **Penman-Monteith** combination **equation** recommended by FAO (Monteith, 1981, 1990).

Print Information
- Print Options: Leave as Default
- Number of Print Times: 12
- *Button* “Select Print Times”
- *Button* “Default”
- *Button* “OK”
- *Button* “Next”

Water Flow – Iteration Criteria
- Leave default values
- *Button* “Next”

Water Flow – Soil Hydraulic Model
- Check Single Porosity Model, van Genuchten – Mualem (default)
- *Button* “Next”

Water Flow – Soil Hydraulic Parameters
- Soil Loam from the Soil Catalogue (default)
- *Button* “Next”

Water Flow – Boundary Conditions
- Upper Boundary Condition: Atmospheric BC with Surface Run Off
- Lower Boundary Condition: Free Drainage
- Initial Condition: In Pressure Heads
- *Button* “Next”

Root Water and Solute Uptake Model
- Water Uptake Reduction Model
- Check Feddes (Default)
- *Button* “Next”

Root Water Uptake Parameters
- Select Pasture from the Database (default)
- *Button* “Next”

Time-Variable Boundary Conditions

Prepare the precipitation time series in a spreadsheet, select the first cell in the 'Time' column and then paste values from the spreadsheet using the Ctrl+V keyboard command. The time series of rainfall data is displayed in Figure 4.1.

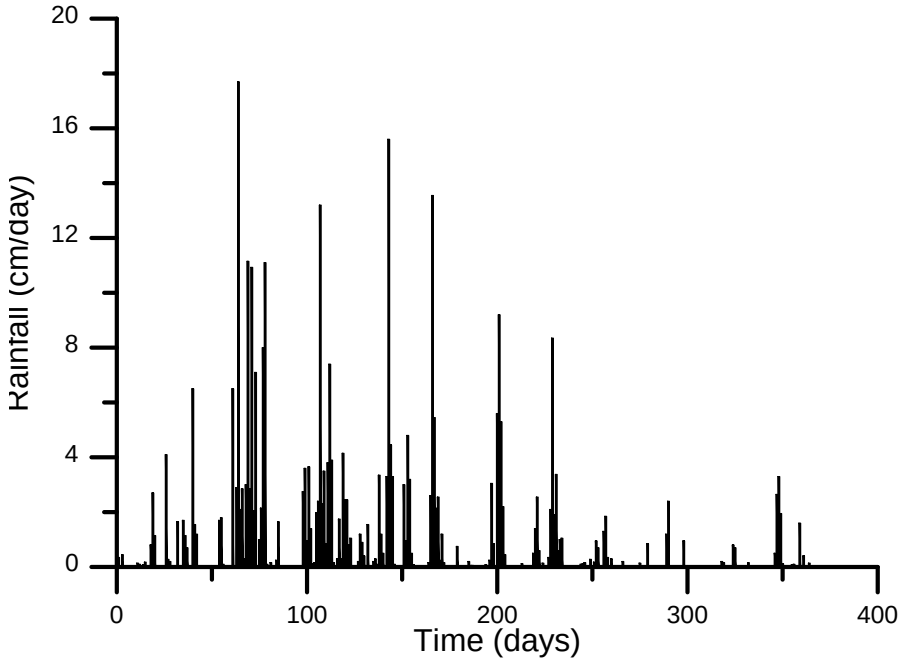

Figure 4.1. Time series with daily rainfall values.

Meteorological Parameters

In the **Meteorological Parameters** dialog window (Fig. 4.2), users specify parameters needed to calculate potential evapotranspiration using either the Penman-Monteith or Hargreaves equations, using geographical and meteorological parameters, and parameters related to crop growth, *LAI*, and interception. You must then specify **Latitude** (deg) and **Altitude** (m), **Angstrom values** a_s (recommended value is 0.25) and b (recommended value is 0.5), values a_1 (recommended value is 0.9) and b_1 (recommended value is 0.1) for calculating **the effect of a cloudiness factor on long wave radiation**, values a_l (recommended value is 0.34) and b_l (recommended value is –0.139) for calculating **the effect of emissivity on long wave radiation**, and heights of wind speed and temperature and humidity measurements (usually 200 cm) (see Chapter 2.7 for details).

You must also specify whether or not a crop is present. If a crop is present, then the crop data may be constant in time or must be entered. If the latter, data can be entered via a **table** (the data are then interpolated linearly in time between entered values) or can be provided in terms of **daily values**. Relevant **crop data** are Crop Height, Albedo, LAI, and RootDepth. When "No Crop" is selected, a (surface) Albedo has to be provided. A default value of Albedo for simulations with a crop is 0.23.

If the **Crop Data Daily** option is selected in the **Meteorological Parameters** window, then the **Crop Height** and **Root Depth** need to be specified at the same times as other

Meteorological variables. If **Crop Data** in **Tables** is selected, then **Crop Height** and **Root Depth** should be specified at selected times in the **Growth Data** table.

Users must also specify how *LAI* is calculated. *LAI* can be calculated from:

a) **From Crop Height, Clipped Gras**: the crop height combined with a formula for grass (i.e., *LAI* = 0.24×CropHeight),
b) **From Crop Height, Alfalfa:** the crop height combined with a formula for alfalfa (i.e., *LAI* = 1.5×log(CropHeight)+5.5), or
c) **From Surface Fraction**: based on the surface cover fraction, *SCF*, (i.e., $LAI = -1/a_i \times \ln(1-SCF)$, where a_i is the constant for the radiation extinction by the canopy [-] = 0.463).

- Enter values as shown below in Figure 4.2. Note that the geographical parameters refer to the Tully region in north Queensland, Australia.
- *Button* "Next"

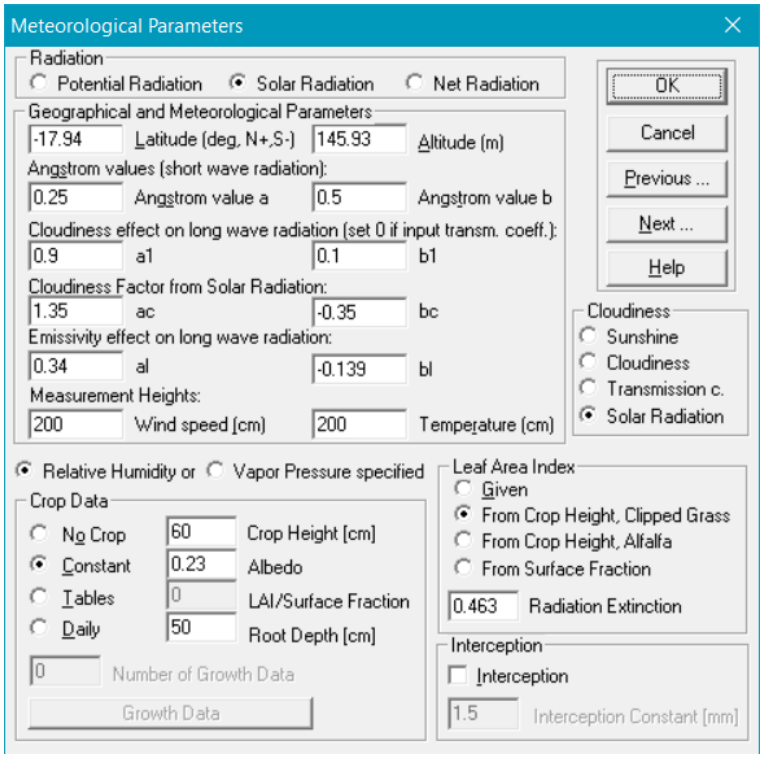

Figure 4.2. The **Meteorological Parameters** dialog window.

Meteorological Conditions

- Prepare the time series for solar radiation (Radiation), maximum (T_max) and minimum (T_min) daily air temperatures, relative humidity or vapor pressure (Humidity), and wind speed (Wind) in a separate spreadsheet, select the first cell in the 'Time' column of the **Meteorological Conditions** dialog window (Fig. 4.3) and then paste values from a spreadsheet using the Ctrl+V keyboard command.
- *Button* "Next"

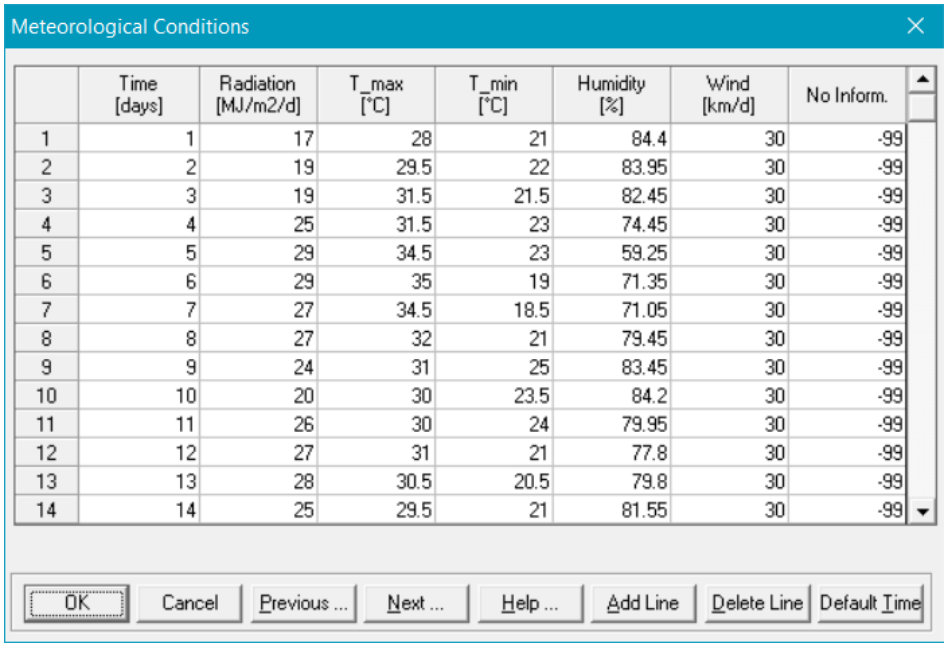

Figure 4.3. The **Meteorological Conditions** dialog window.

HYDRUS-1D guide

- Do you want to run PROFILE application?
- *Button* "OK"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Root Distribution or **Toolbar** 
- Click the "Edit Condition" button (left side), select with the Mouse the nodes down to a depth of 50 cm, left click the mouse again, in the **Condition Specification** dialog window that appears enter *Roots Linear Distribution*: Top value=1, check 'Use top value for both', and click the OK button. This means that roots are distributed uniformly in the top 50 cm of the soil profile (according to the Feddes model in Figure 3.3).
- **Menu**: Conditions->Observation Nodes or **Toolbar** 
- Click the "Insert" *Button* on the left-side Edit Bar and specify nodes at 50 and 100 cm (right-click to end the command)
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Profile Information

- Figure 4.4 shows two pressure head profiles at 152.5 (black line) and 335.5 (red line) days, which represent conditions after a wet and a dry period, respectively. Note that the pressure head in the top 50-cm root zone drops to P3 (the wilting point, -8,000 cm for pasture) after the dry period,
- Figure 4.5 shows two corresponding flux profiles at 152.5 and 335.5 days. Note a much higher flux following the wet period and almost a zero flux along most of the root zone following the dry period.

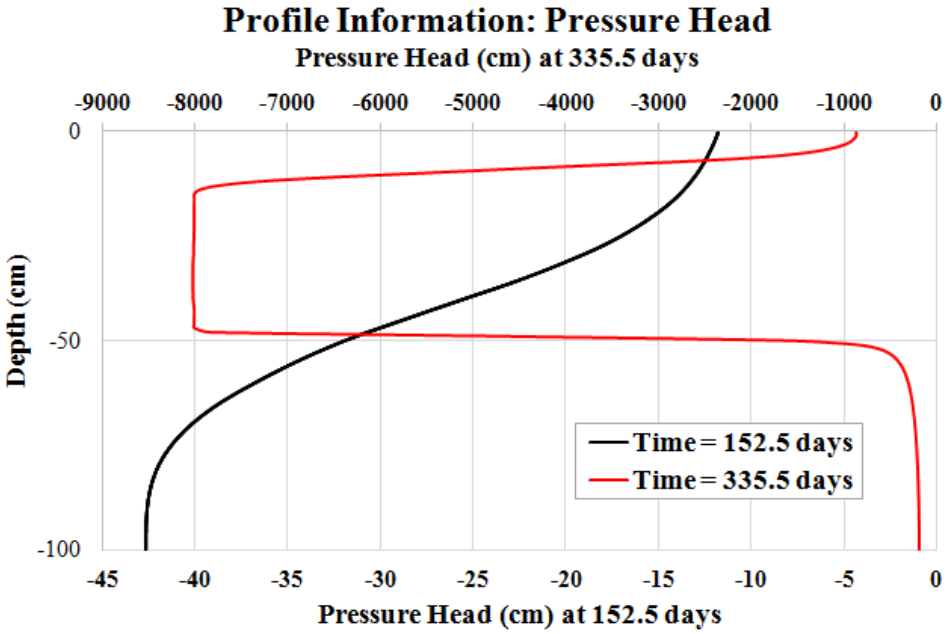

Figure 4.4. Pressure head profiles at two selected times.

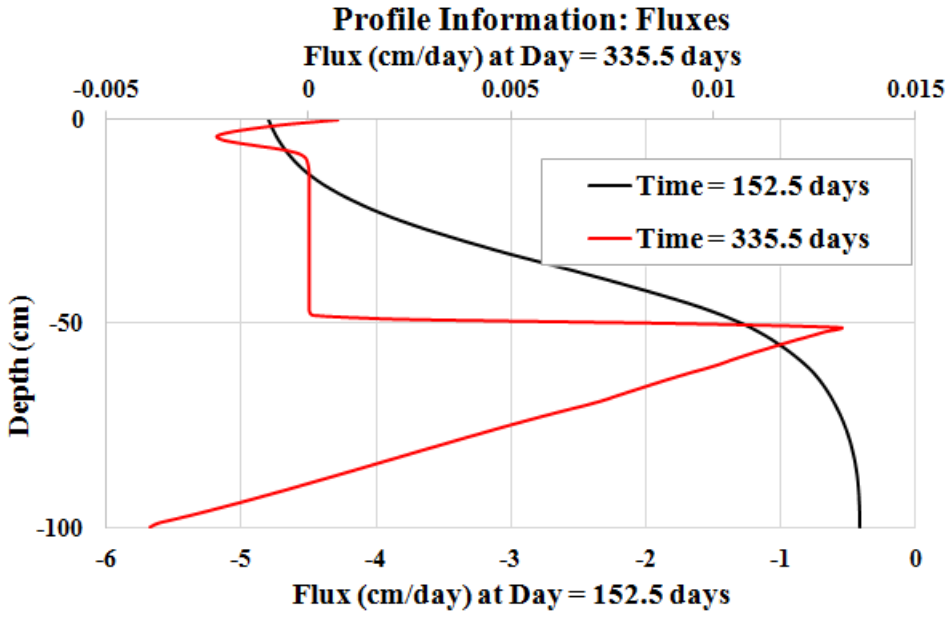

Figure 4.5. Flux profiles at two selected times.

Water Flow - Boundary Fluxes and Heads

- Figure 4.6 shows the estimated potential root water uptake rates derived from the meteorological data. Note the seasonal signal, which reflects lower uptake during winter (which in the southern hemisphere is around July).
- Figure 4.7 shows actual root water uptake (compare actual uptake with potential uptake (Fig. 4.6) and the actual surface flux due to infiltration of precipitation (Fig. 4.8)). Note that actual root water uptake (transpiration) is significantly smaller during periods without precipitation or immediately after large rainfalls.
- Figure 4.9 shows the actual bottom flux, which represents deep drainage that occurs below the root zone. This flux will continue downwards by gravity until it eventually recharges the underlying aquifer. Note that most of the recharge corresponds to large rainfall events when the soil profile is saturated (and highly conductive).
- Figure 4.10 shows the cumulative fluxes; the actual surface flux (infiltration minus evaporation) is negative (downward) and represents infiltration, the actual bottom flux is negative (outflow) and represents recharge, and the actual root water uptake (transpiration) is positive (upward). Note that the magnitude of the surface flux is about equal to that of the root water uptake flux and the bottom flux.
- If one is interested in the time history of groundwater recharge, i.e., when the aquifer is actually recharged, one would need to model the entire soil profile down to the water table. In the current example, only the first 100 cm of a deep unsaturated zone are considered.

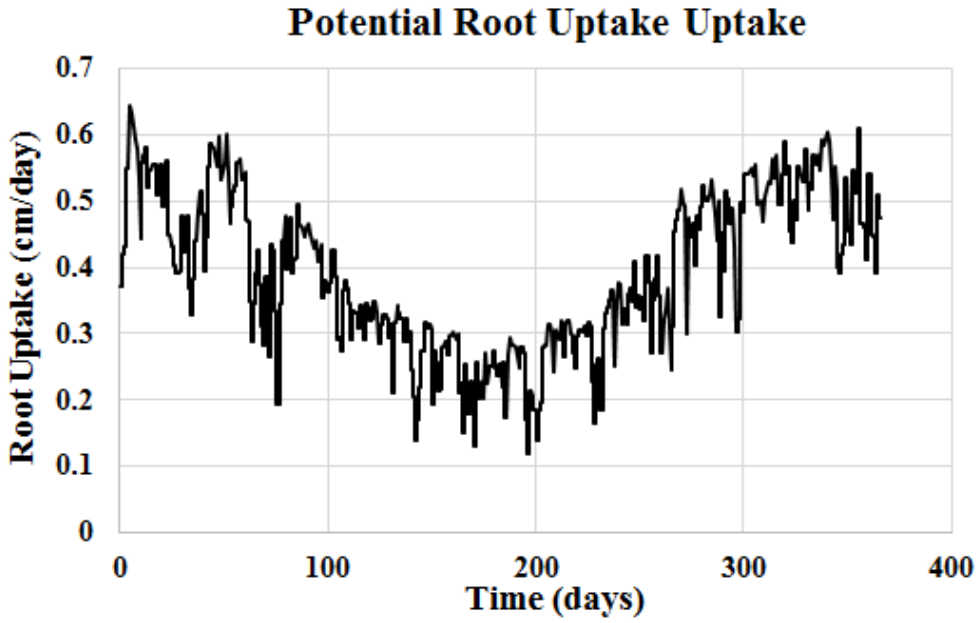

Figure 4.6. Potential root water uptake versus time.

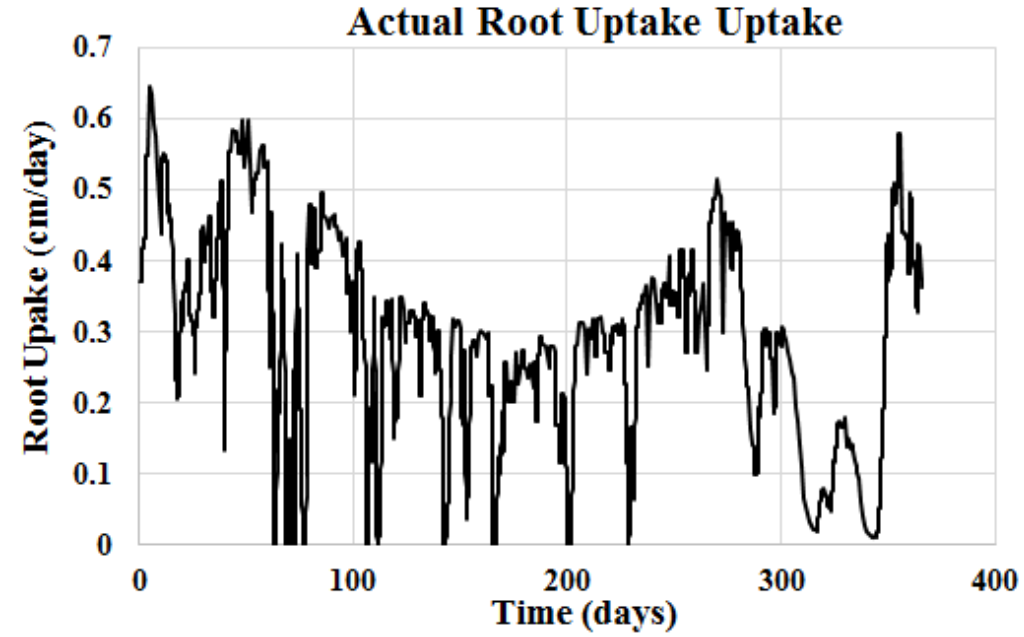

Figure 4.7 Actual root water uptake versus time.

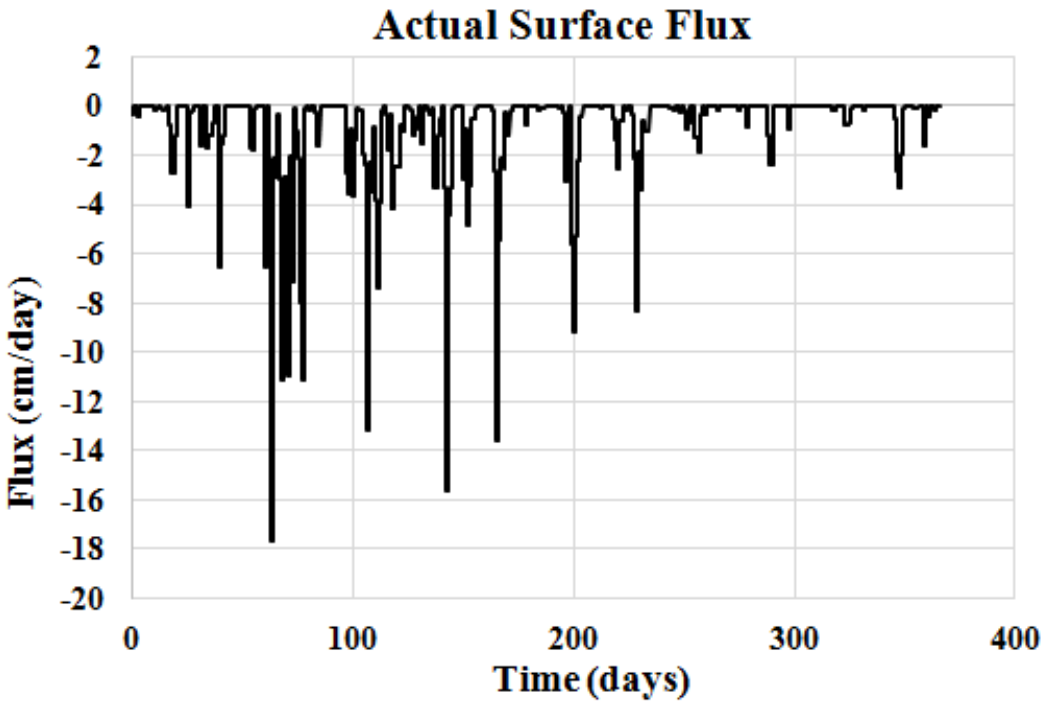

Figure 4.8. Actual surface flux (into the soil profile) versus time.

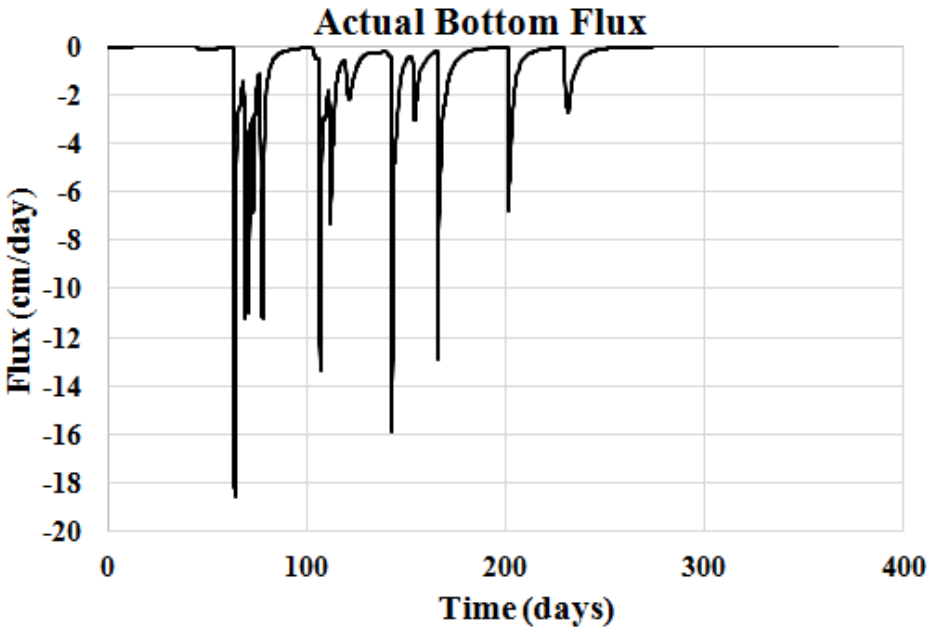

Figure 4.9. Actual bottom flux (out of the soil profile) versus time.

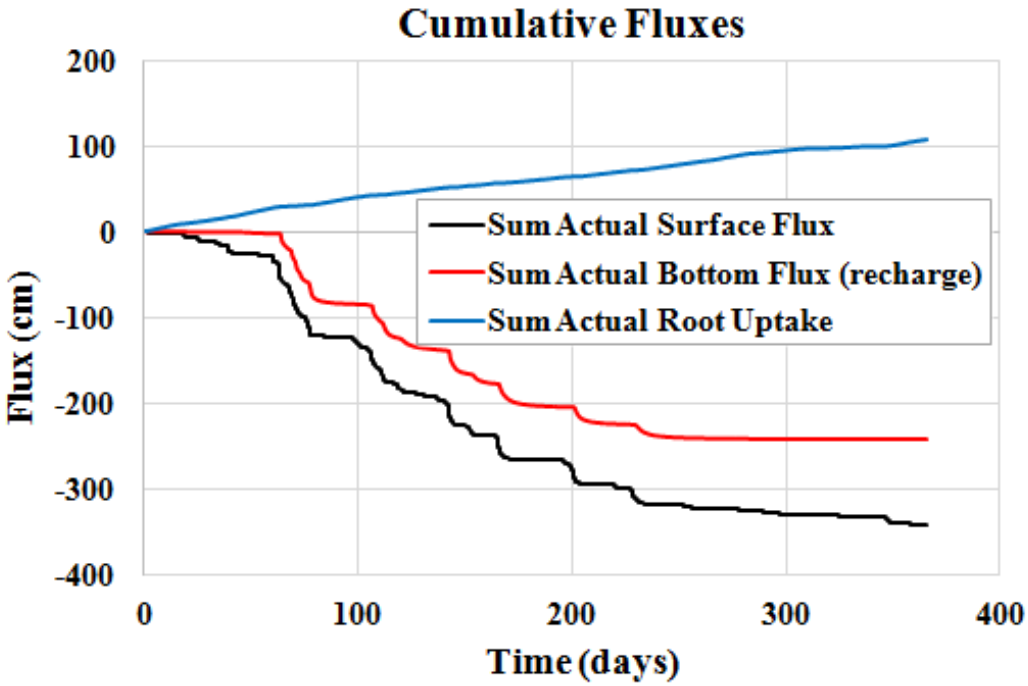

Figure 4.10. Cumulative actual (surface, bottom, and transpiration) fluxes versus time.

Example 5a: Basic Solute Transport: Solute Introduced through a Constant Flux Boundary

Example Description and Objectives

The objective of Example 5a is to provide an introductory example involving solute transport under variably-saturated flow conditions. Water flow and solute transport through a 300-cm deep uniform soil profile with an initial pressure head of -100 cm (the default initial value in HYDRUS-1D) is simulated in this example. The soil profile is initially solute free. Water infiltrates into the soil profile at a constant flux of 5 cm/d during the entire 20-day simulation. Infiltrating water has a unit solute concentration during the first 10 days and is solute free during the second 10 days. Water and solute drain through the bottom 'Free Drainage' boundary.

This example demonstrates how solute is introduced into the soil profile using a flux boundary and how solute breaks through at various locations in the soil profile. The numerical stability criteria and dimensionless Peclet and Courant numbers (Perrochet and Berod, 1993) are also discussed.

Pre-Processing

Project Manager
- Select the *Projects* Tab
- Button "New"
- Name: Example 5a
- Description: Basic Solute Transport - Solute through a flux boundary
- *Button* "OK"

Main Processes
- Heading: Solute through a flux boundary
- Check "Solute Transport" (in addition to "Water Flow", which is checked by default)
- *Button* "Next"

Geometry Information
- Depth of Soil Profile (cm): 300 cm
- *Button* "Next"

Time Information
- Time Discretization:
- Final Time (day): 20
- *Button* "Next"

Print Information
- Print Options: Leave as default
- Number of Print Times: 10
- *Button* "Select Print Times"
- *Button* "OK"
- Print Times: Leave default values

- *Button* “Next”

Water Flow – Iteration Criteria
- Leave default values
- *Button* “Next”

Water Flow – Soil Hydraulic Model
- Leave as default (Single Porosity, van Genuchten – Mualem)
- *Button* “Next”

Water Flow – Soil Hydraulic Parameters
- Leave as default (parameters for Loam)
- *Button* “Next”

Water Flow – Boundary Conditions
- Upper Boundary Condition: Constant Flux
- Lower Boundary Condition: Free Drainage
- Initial Condition: In Pressure Heads
- *Button* “Next”

Water Flow – Constant Boundary Fluxes
- Upper Boundary Flux: -5 (cm/d; note that negative fluxes are downwards; the ratio of water flux to the saturated hydraulic conductivity is 0.2, i.e., the soil remains unsaturated)
- *Button* “Next”

Solute Transport - General Information

The next set of four dialog windows deals with solute transport. In the **Solute Transport** dialog window (Fig. 5a.1), you can select a time and space weighting discretization scheme (although using the default schemes, i.e., the Crank-Nicholson Scheme with Galerkin Finite Elements, is recommended). For minimizing or eliminating numerical oscillations, HYDRUS-1D implements the combined Peclet and Courant number criterion introduced by Perrochet and Berod (1993), with a recommended default stability criterion of 2. In other words, when the combined effect of Peclet and Courant number is less than or equal to 2 ($Pe \times Cr \leq 2$), numerical oscillations in the solute transport solution should be minimal. Further details about the time and space weighting scheme are discussed in Appendix I.

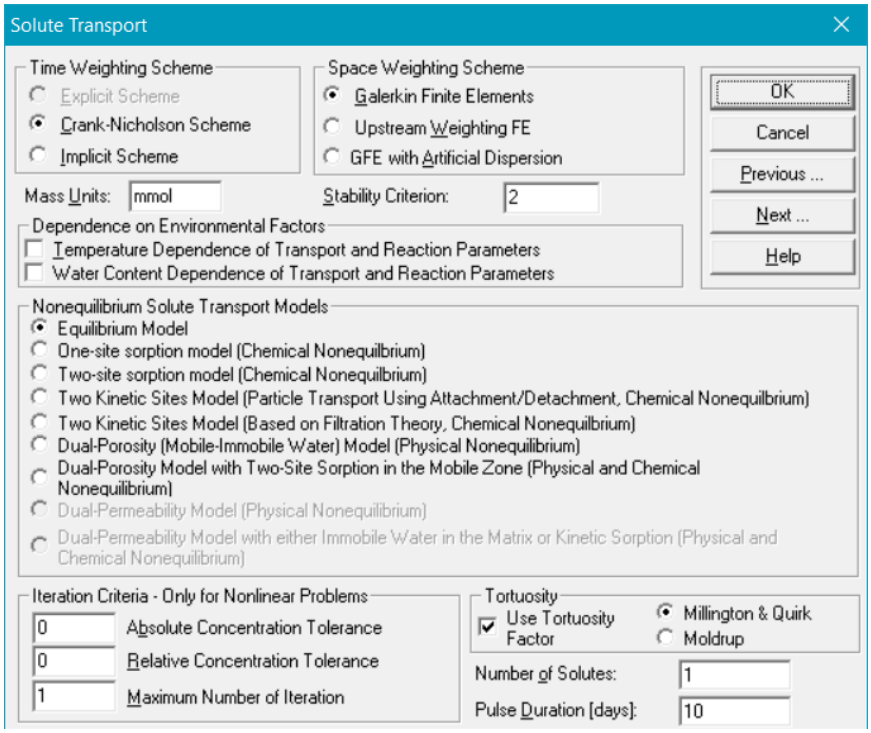

Figure 5a.1. The **Solute Transport** dialog window.

The next option available is about whether the solute transport and reaction parameters are water content and/or temperature dependent (in the "Dependence on Environmental Factors" section). Indeed, several of the diffusion, zero-order production, first-order degradation, and adsorption coefficients may be strongly dependent upon temperature (Chapter 3.4). This could also be relevant when the Major Ion Chemistry module (not discussed here) is invoked to calculate carbon dioxide transport and production or multi-component chemistry related to saline and/or sodic soils (see Chapter 5). The water content dependence of degradation coefficients is implemented using a modified equation of Walker (1974); if this option is selected, two parameters need to be provided (Figure 5a.): a solute dependent parameter B (usually 0.7), and a reference pressure head (h_{ref}) which defines the reference water content (θ_{ref}) at which the reference degradation constant (a_r) is defined. Water content dependent degradation rates have been reported for denitrification (Morales et al., 2016) and carbon (Jacques et al., 2018; Sierra et al., 2012) cycling. In the current example, neither the temperature nor the water content dependence option is activated.

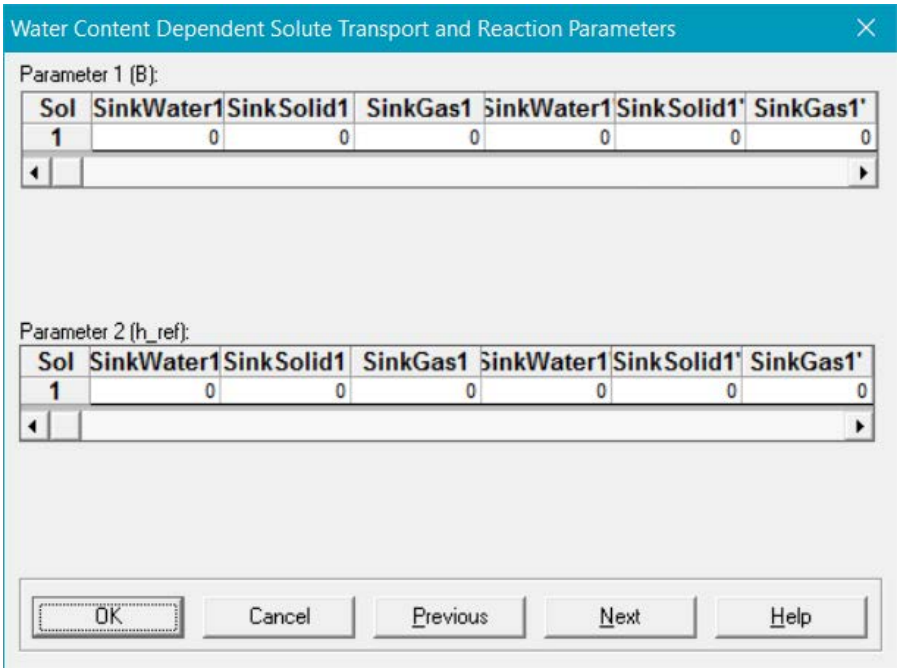

Figure 5a.2. The Water Content Dependent Solute Transport and Reaction Parameters dialog window.

The next options are about invoking the nonequilibrium solute transport model (in the "Nonequilibrium Solute Transport Models" section). Note that the default option is the equilibrium model. Solute transport in that case occurs in the full water-filled pore space (i.e., only a mobile flow region exists), while solute partitioning between the liquid and solid phase is assumed to instantaneous (i.e., not kinetically controlled). Details of the different nonequilibrium models are described in Chapter 3 and Šimůnek and van Genuchten (2008).

When solute transport is nonlinear (e.g., when nonlinear sorption is considered), you need to specify "Iteration Criteria" for the solution of the solute transport equation.

You also have an option to select whether the "Tortuosity Factor" in the diffusion coefficient for the water and gas phases should be considered and whether the Millington and Quirk (1961) or Moldrup (Moldrup et al., 2000) model should be used for this (Table 5a.1). If the "Tortuosity Factor" option is not used, the model uses a default value of one for the tortuosity factor. This means that the effective diffusion coefficient for the water phase ($D_{p,w}$) is equal to the free water diffusion coefficient (D_w):

$$D_{p,w} = D_w \tau_w = D_w \quad \text{if} \quad \tau_w = 1 \tag{5a.1}$$

while the pore diffusion coefficient for the gas phase ($D_{p,g}$) is defined as

$$D_{p,g} = \frac{D_g \tau_g a_v}{\theta} = \frac{D_g k_g a_v}{\theta} \quad \text{if} \quad \tau_g = 1 \tag{5a.2}$$

where D_g is the diffusion coefficient in the gas phase, a_v is volumetric air content (cm^3/cm^3) and k_g is the inverse of the Ostwald coefficient ($1/k_g = K_H R_u T^A$, where K_H is the Henry's Law constant ($mol/(atm \times m^3)$), R_u is the universal gas constant (8.31451 m^2 kg s^{-2} mol^{-1} K^{-1}), and T^A is absolute temperature (degree K). Values for free water diffusion coefficient (D_w) are listed in Table 5a.2 for a number of common chemicals (about 1.7 cm^2/d for Cl). A good reference publication on solute diffusion coefficients is Flury and Gimmi (2002). Typical values for the diffusion coefficient in the gas (air) phase (D_g) are 20,000 cm^2/day for CO_2 (Jacques et al., 2018), 8,640 cm^2/day for radon (Sϕgaard-Hansen and Damkjaer, 1987), and 16,940 cm^2/day for methane (Marrero and Mason, 1972).

Table 5a.1. Tortuosity factors for the water (τ_w) and gas (τ_g) phases. Other parameters are the water content (θ), the saturated water content (θ_s), and the volumetric air content (a_v).

Tortuosity model	Water phase	Gas phase
Millington-Quirk (1961)	$\tau_w = \frac{\theta^{7/3}}{\theta_s^2}$	$\tau_g = \frac{a_v^{7/3}}{\theta_s^2}$
Moldrup et al. (2000)	$\tau_w = 0.66\left(\frac{\theta}{\theta_s}\right)^{8/3}$	$\tau_g = \frac{a_v^{1.5}}{\theta_s}$

Table 5a.2. Diffusion coefficients in free water at 18°C, D_w (source: Li and Gregory, 1974).

Chemical	D_w (cm^2/day)
Cations	
H^+	7.06
Na^+	0.98
K^+	1.44
Mg^{2+}	0.51
Ca^{2+}	0.58
Anions	
OH^-	3.88
Cl^-	1.48
HCO_3^-	1.02
SO_4^{2-}	0.77
PO_4^{3-}	0.53

Users can further specify how many solutes will be considered in the advective-dispersive transport equations (one equation per solute will then be solved). Up to 10 solutes can be defined. Finally, you can specify for how long ("Pulse Duration") solute is applied at (or released from) the soil surface. Use this option only when constant water flow boundary conditions are used at the soil surface.

- Leave everything as default, except
- Pulse Duration [day]: 10 (solute will be applied during the first 10 days, while solute-free solution will be applied after that)
- *Button* "Next"

Solute Transport - Transport Parameters

The next dialog window is used to specify general solute transport parameters. In the **Solute Transport Parameter** dialog window (Fig. 5a.3) you can specify such parameters as the bulk density, the dispersivity (e.g., Vanderborght and Vereecken, 2007), and diffusion coefficients for solutes in both the liquid phase (see Table 5.a.2 for examples) and the gas phase if volatile solutes are present. If the "Use Tortuosity Factor" option is activated, the liquid ("Diffus. W.") and gas ("Diffus. G.") diffusion coefficients should be the free water (D_w) and air phase (D_g) diffusion coefficients. Alternatively, if the "Use Tortuosity Factor" option is not activated, the tortuosity is equated to one and the diffusion coefficients entered should be the pore diffusion coefficients for the water ($D_{p,w}$) and gas ($D_{p,g}$) phases.

The two parameters "Frac" and "ThIm" are used only with nonequilibrium solute transport models and should be equal to 1 and 0, respectively, for equilibrium solute transport (i.e., transport without preferential flow and kinetically controlled sorption).

- Leave as default
- Note that Disp. = 30 cm, i.e., one-tenth of the travel distance, which is 300 cm.
- Note that the molecular diffusion coefficient in the liquid phase (Diffus.W.) is set equal to zero. This process is often neglected since in the majority of applications it is significantly smaller than hydrodynamic dispersion. On the other hand, it is possible to set this value equal to about 1 cm^2d^{-1}, which is an approximate value for a majority of solutes.
- *Button* "Next"

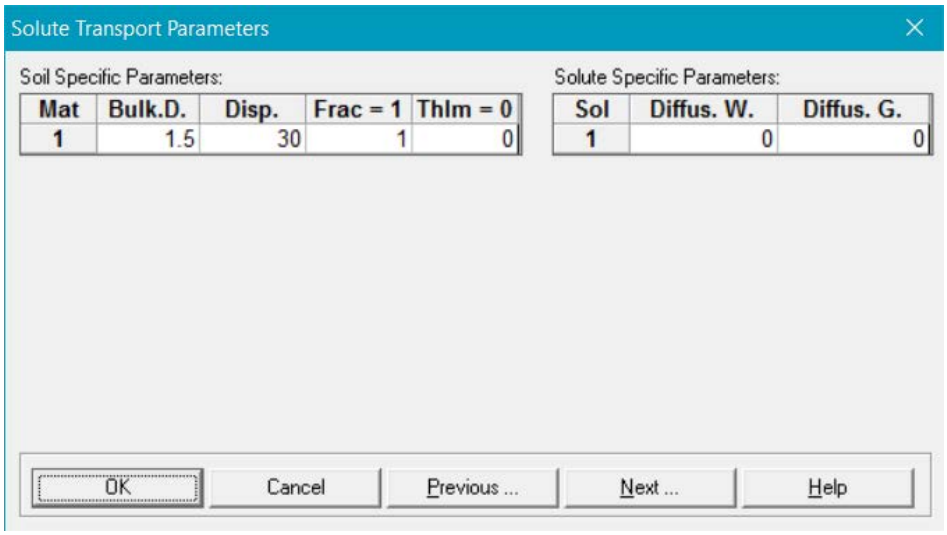

Figure 5a.3. The **Solute Transport Parameters** dialog window.

Solute Transport - Reaction Parameters

The **Solute Transport and Reaction Parameter** dialog window (Fig. 5a.4) is used next to specify parameters for various chemical and biological processes such as sorption (K_d, *Nu*, *Beta*), Henry's law constant (*Henry*) for volatile substances, and several degradation constants (e.g., *SinkWater1*, *SinkSolid1*, *SinkGas1*, *SinkWater0*, etc). Degradation rates can be in the form of zero- and first-order processes and need to be specified for each phase (i.e., liquid, solid, and gaseous) separately. The default values are all zero. When identifying degradation rates, you need to pay close attention to how the values (e.g., half-lives) are reported. They may be reported for each individual phase (again, either liquid, solid, or gaseous), or for the entire (multi-phase) system. For details see Chapter 3 (or press F1).

- Leave as Default
- Note that all parameters are equal to zero except for the Freundlich exponent, which is equal to 1, i.e., parameters are set for a nonreactive tracer
- *Button* "Next"

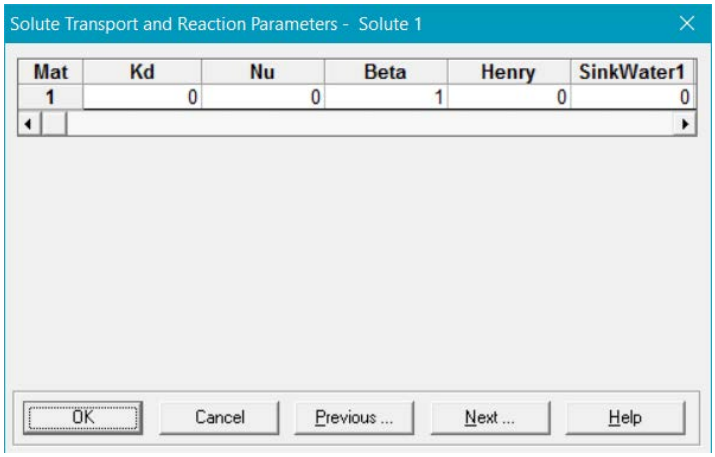

Figure 5a.4. The **Solute Transport and Reaction Parameters** dialog window.

Solute Transport - Boundary Conditions

Next, you need to specify appropriate boundary conditions for solute transport to define how the soil profile interacts with the outside environment (i.e., at the upper and lower boundaries). This is done using the **Solute Transport Boundary Condition** dialog window (Fig. 5a.5).

- Leave as Default
  (i.e., Upper Boundary Condition: Concentration Flux BC;
  Lower Boundary Condition: Zero Concentration Gradient)
  For more details on solute transport boundary conditions, refer to Appendix II.2
- Boundary Condition for Solute 1: 1 (this is the concentration of the infiltrating water, in mmol/cm^3)
- *Button* "Next"

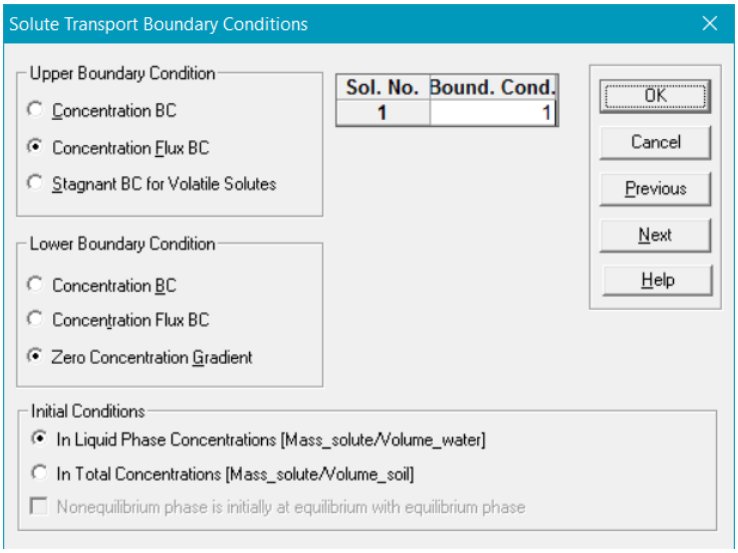

Figure 5a.5. The **Solute Transport Boundary Conditions** dialog window.

HYDRUS-1D guide

- Do you want to run PROFILE application?
- *Button* "OK"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Observation Nodes or **Toolbar**
- *Button* (left side) "Insert": select nodes at 0, 150, and 300 cm
- **Menu**: File->Save Data or **Toolbar**
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button.

Post-Processing

Observation Points

Referring to Figure 5a.6:

- The concentration at the surface (ON-1) increases during the first 10 days while the solute pulse is active at the upper Constant Flux boundary. Solute (1 mmol/cm^3) was applied during the first 10 days only (see Figure 5.a.2), but the concentration never reaches unity. Had the pulse continued indefinitely, the entire profile would have attained a unit concentration. However, owing to the low infiltration rate, it takes a rather long time for the soil in this example to reach a steady-state water content and to replace the initially solute free soil solution with 1 mmol/cm^3 infiltrating solution). The concentration declined as the solute-free water infiltrates the profile after day 10.

- The concentration at a depth of 150 cm (ON-2) reached 0.36 mmol/cm^3 after 10 days. Even though solute-free water infiltrated after day 10, the concentration continued to increase until it peaks at 0.58 mmol/cm^3 as flowing water continues to carry solutes downward from the soil above this observation point. The soil above this point has a higher concentration.
- The solute breaks through at the bottom of the profile (ON-3)) after about 9 days.
- Had solute-free water continued to infiltrate the profile indefinitely, all solute would eventually be leached out of the profile, thus returning the soil column to its initial state.

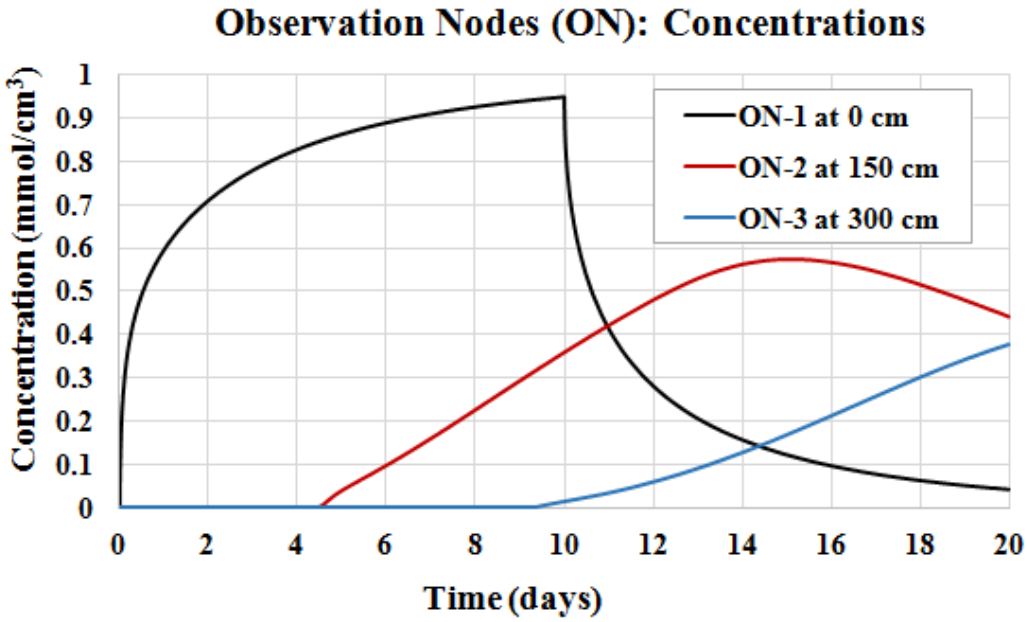

Figure 5a.6. Solute concentrations versus time at selected observation points.

Profile Information

Referring to Figure 5a.7:

- Note the declining concentration peak along the depth of the profile due to solute dispersion.
- Note that at 10 d, the concentration at a depth of 300 cm (the lower boundary) is just above zero, indicating that solute has just broken through this boundary (Figure 5a.6).
- If the area under each curve is integrated, we should get the total solute mass stored within the soil profile at that particular time. This value is reported as 'ConcVol' in the 'Mass Balance Information'.

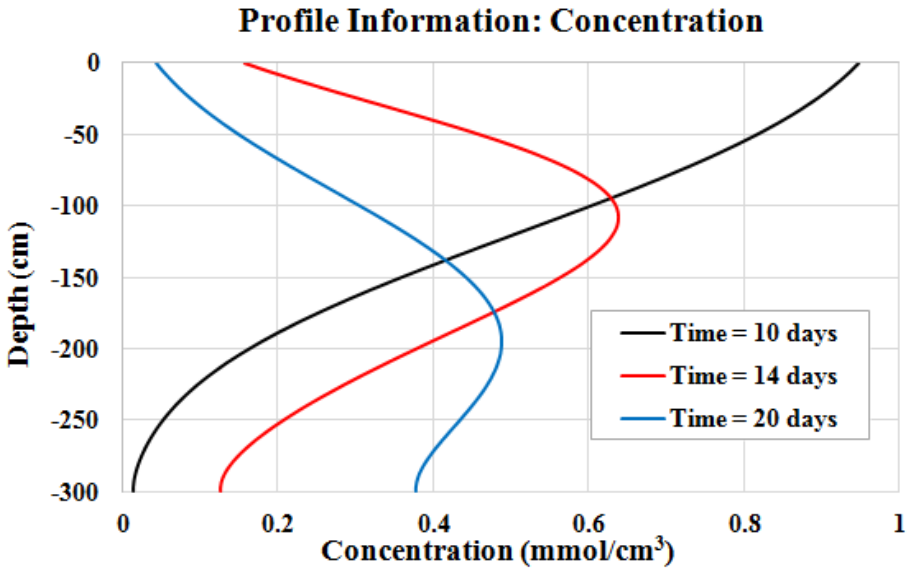

Figure 5a.7. Concentration profiles at selected times.

Solute Fluxes

Referring to Figure 5a.8:

- Note that solute fluxes are positive when entering the transport domain and negative when leaving the transport domain. This is different than those for water flow, which are always positive upwards and negative downwards.
- The cumulative solute flux entering the soil profile through the upper atmospheric boundary peaks at 50 mmol/cm^2. This because a unit concentration was present in the precipitation, which entered the profile at a rate of 5 cm/day for 10 days (i.e., 1 mmol/cm^3 × 5 cm/day × 10 days =50 mmol/cm^2).
- The sum of the influx and efflux curves at any time defines the amount of solute stored within the soil profile. This value is reported as 'ConcVol' in the 'Mass Balance Information' (e.g., 41.27 mmol/cm^{2}at day 20, which is equal to the cumulative surface flux + the cumulative bottom flux).

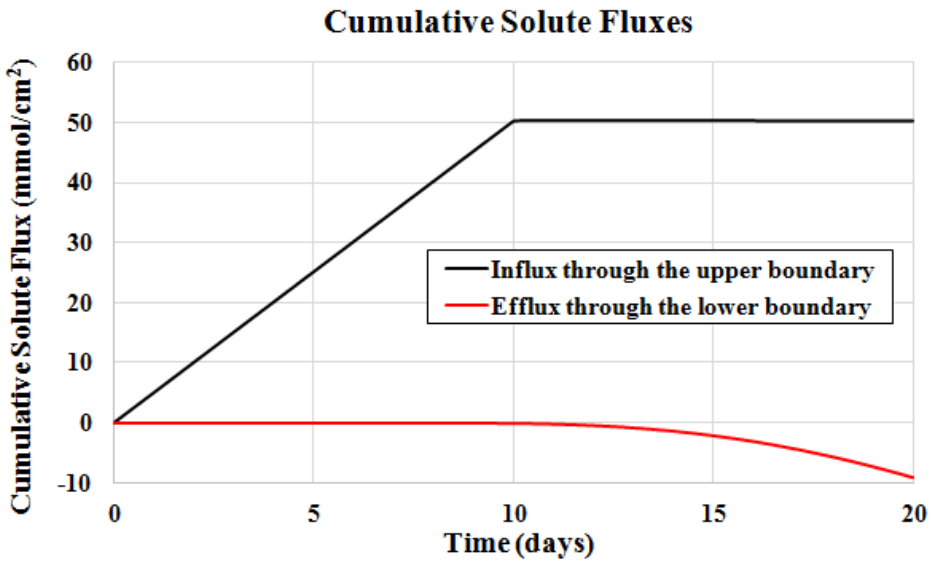

Figure 5a.8. Cumulative solute fluxes (into and out of soil profile) versus time.

Run Time Information

- The grid Peclet number (Pe) defines the predominant type of the solute transport (the ratio of the advective and dispersive transport terms) in relation to the coarseness of the finite element grid. The Peclet number increases when the advective component of the transport problem dominates the dispersive part, which is exhibited by a steep concentration front. To achieve acceptable numerical results, the spatial discretization must be kept relatively fine to maintain a low Peclet number (smaller than 2). Figure 5a.9 shows a low Peclet number throughout the simulation, which indicates a stable simulation.
- The second dimensionless number, which characterizes the relative extent of numerical oscillations, is the Courant number (Cu), which is associated with the time discretization and should be kept below 1 (which the program automatically does).
- A stable HYDRUS-1D simulation maintains the product of these two dimensionless numbers (i.e., the Peclet and Courant numbers) to be under 2. For more details, refer to the HYDRUS-1D Technical Manual (Chapter 8.4.5).

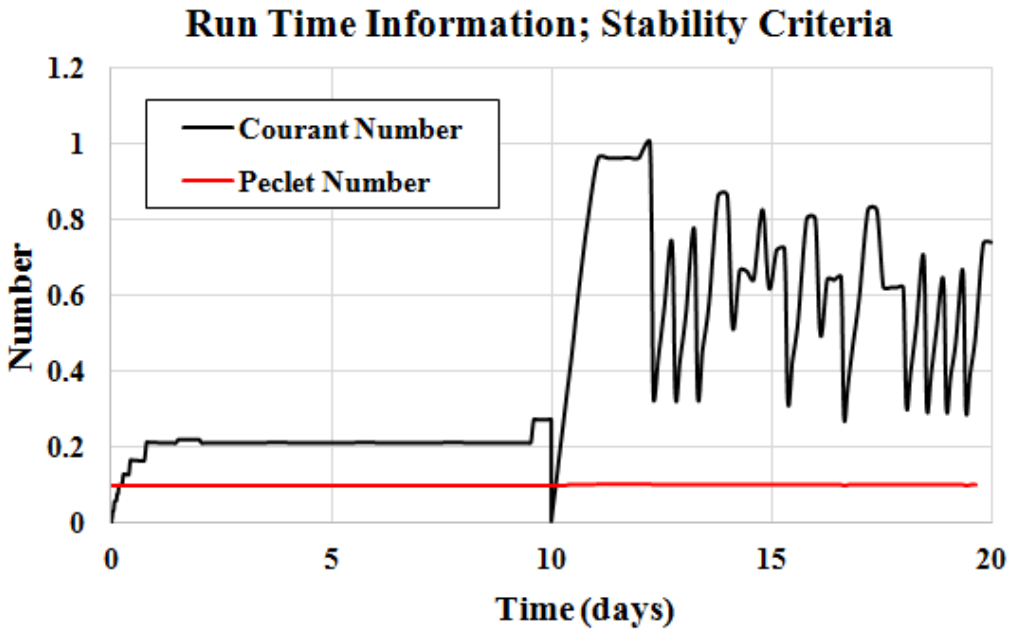

Figure 5a.9. The Peclet and Courant numbers (which are related to stability criteria) versus time.

Example 5b: Basic Solute Transport: Solute Introduced through a Constant Pressure Head Boundary

Example Description and Objectives

This example is the same as Example 5a, except that the constant flux upper boundary is replaced by the constant pressure head boundary. The objective of Example 5b is thus to simulate water flow and solute transport through a 300-cm deep uniform soil profile with an initial pressure head of -100 cm. The soil profile is initially solute free. Water infiltrates into the soil profile through a constant head boundary (0 cm) during the entire 20-day simulation period. Infiltrating water has a unit solute concentration during the first 10 days and is solute free during the second 10 days. Water and solute drains through the bottom 'Free Drainage' boundary.

This example demonstrates how solute is introduced into the soil profile using a constant pressure head boundary and how solute breaks through at various locations in the soil profile. This could be part of a constant-head infiltration experiment where tracers are introduced together with water, a furrow irrigation system providing water and dissolved solutes to a cropped soil (Ebrahimian et al., 2013a,b), water flow processes and the N balance of a rice paddy field (Dash et al., 2015), or a leaking water holding pond introducing a mixture of chemicals into the underlying soil (Mallants et al., 2017).

Pre-Processing

The example is created most easily by simply copying and renaming Example 5a and implementing the required modifications.

Project Manager

- Select the *Projects* Tab
- Select *Example 5a*
- Button "Copy"
- New Name: Example 5b
- Description: Basic Solute Transport - Solute through a flux boundary
- *Button* "OK"
- Select *Example 5b*
- Button "Open"

Since the problem is almost identical as Example 5a (except for the water flow boundary condition), we can skip a large number of input dialog windows and start directly with the **Water Flow Boundary Conditions**. Note that the Solute Boundary Condition is identical to the previous example, i.e., a Concentration Flux Boundary.

Water Flow – Boundary Conditions

- Upper Boundary Condition: Constant Pressure Head
- *Button* "OK"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar**  .

- *Button* (left side) “Edit Condition”: Select with the Mouse the first node, left click the mouse, and specify a pressure head of 0 cm.
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

Referring to Figure 5b.1:

- The concentration at the surface (ON-1) increases during the first 10 days while the solute pulse is active at the upper Constant Pressure Head boundary. However, contrary to Example 5a, the surface concentrations do reach unity. This because under the constant head flow boundary condition the soil becomes saturated quickly and thus the initially solute-free solution near the soil surface is displaced quickly. Similarly, the concentration declines at a much faster rate and all solute is washed out at this location when solute-free water infiltrates into the profile at about day 15. The same applies to (ON-2).
- The solute breaks through at 300 cm depth after only 2 days (compared to 9 days in Example 5a). This is due to the much larger water flux that is now infiltrating into the soil profile through the Constant Pressure Head boundary. To be exact, the water flux q under the constant pressure head is five times larger than under the Constant Flux boundary (q=0.2×K_s for the previous and q=K_s for the current example). Except at very early times (<0.1 day), the actual surface flux is approximately equal to the saturated hydraulic conductivity of the soil (about 25 cm/day), which is five times the constant flux applied in Example 5a.

Profile Information

Referring to Figure 5b.2:

- Note that after 10 days (the end of the solute pulse), the minimum solute concentration across the entire profile was about 95% of the applied concentration (the profile almost reached a steady-state corresponding to a unit concentration).
- At day 20, the applied solute was almost completely washed out from the upper half of the profile, with little solute remaining in the lower half.

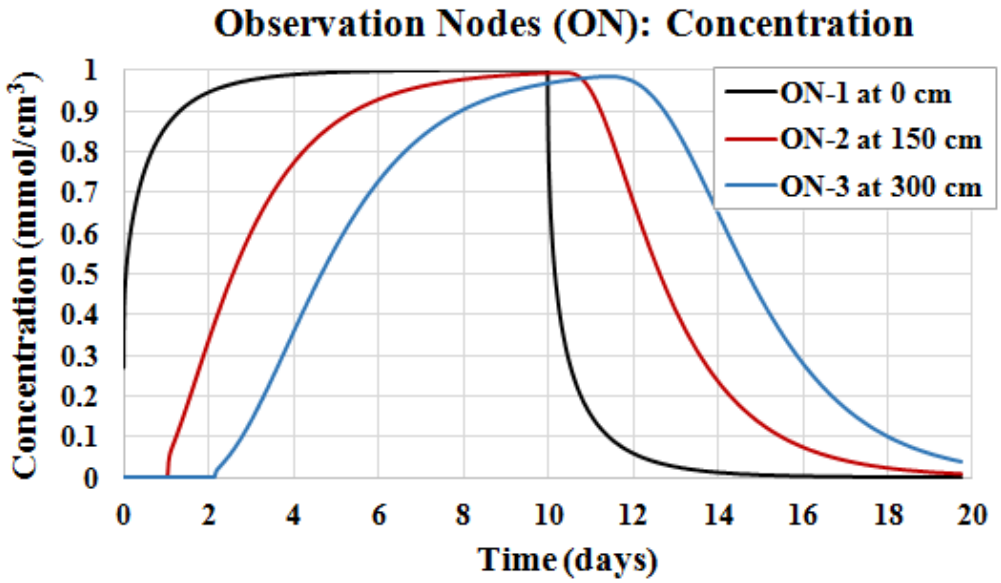

Figure 5b.1. Solute concentrations versus time at selected observation points.

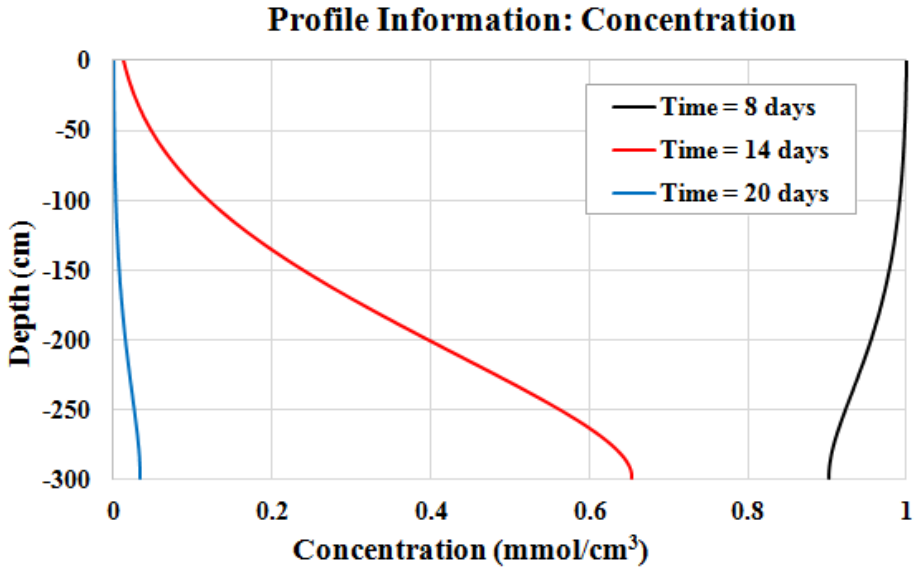

Figure 5b.2. Concentration profiles at selected times.

Solute Fluxes

Referring to Figure 5b.3:

- The cumulative solute mass that infiltrated into the soil profile through the upper Constant Pressure Head boundary was about 250 mmol/cm^2. This follows (approximate) from having a unit concentration, K_s being about 25 cm/day, a having a pulse of 10-day duration (i.e., 1 mmol/cm^3 × 25 cm/day × 10 days = 250 mmol/cm^2).
- The sum of the two curves at any time is the solute stored within the soil profile at that time. At the end of the simulation, the solute mass is equal to about 0.9

mmol/cm^2 (refer to 'ConcVol' in the 'Mass Balance Information' at day 20), which shows that almost all of the solute introduced to the soil profile via the upper boundary has been leached out through the lower Free Drainage boundary.

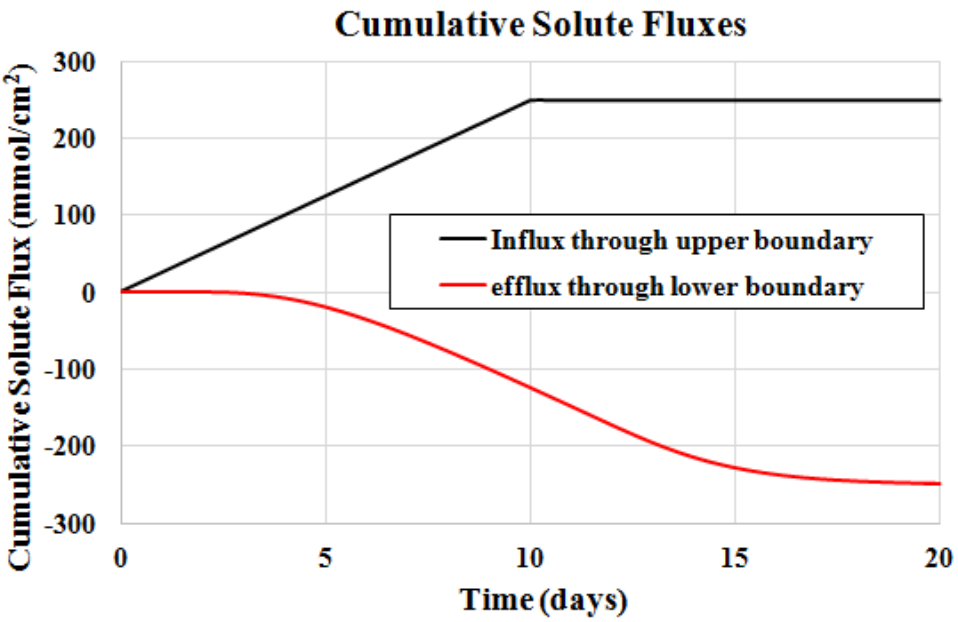

Figure 5b.3. Cumulative solute fluxes into and out of the soil profile versus time.

Example 5c: Basic Solute Transport: Profile with Non-Zero Initial Solute Concentration

Example Description and Objectives

This example is again based on Example 5a, except that solute is now initially present in the top 30 cm of the soil profile and solute-free water infiltrates the soil. Example 5c thus simulates water flow and solute transport through a 300-cm deep uniform soil profile with an initial pressure head of -100 cm. The soil profile has solute mass stored within the top 30 cm (concentration = 30 mmol/cm^3). Solute-free water is introduced through the upper 'Constant Flux' boundary' during the entire 30-day simulation. Water drains through the bottom 'Free Drainage' boundary.

This example demonstrates how solute is mobilized and washed out from the soil profile.

Pre-Processing

You can create this example again by copying and renaming Example 5a and modifying it.

Project Manager

- Select the *Projects* Tab
- Select *Example 5a*
- Button "Copy"
- New Name: Example 5c
- Description: Basic Solute Transport - Solute initially in the profile
- *Button* "OK"
- Select *Example 5c*
- Button "Open"

Main Processes

- Heading: Solute initially in the profile
- *Button* "OK"

Time Information

Time Discretization:

- Final Time (day): 30
- *Button* "Next"

Print Information

- Print Options: Leave as default
- Number of Print Times: 4
- *Button* "Select Print Times"
- Print Times (day): 2, 5, 15, 30
- *Button* "OK"
- *Button* "OK"

Solute Transport - General Information

- Leave as default, except
- Pulse Duration [day]: 30 (a solute-free solution is applied at the boundary)
- *Button* "Next"

Solute Transport - Boundary Conditions

- Leave as Default
  (i.e., Upper Boundary Condition: Concentration Flux BC;
  Lower Boundary Condition: Zero Concentration Gradient)
- Boundary Condition for Solute 1: 0 (a solute-free solution is applied at the boundary)
- *Button* "Next"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Initial Conditions->Concentration or **Toolbar**  and select Concentration 1 from the Quantity listbox on the Edit bar
- *Button* (left side) "Edit Condition": select with the Mouse the upper 30 cm, left click the mouse, and specify the initial solute concentration of 30 (mmol/cm^3).
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

Referring to Figure 5c.1:

- The concentration at the surface (ON-1) rapidly drops as solute-free water infiltrates into the soil profile.
- The initial solute bulge (from 0-30 cm) rapidly disperses and travels down the profile, resulting in a maximum concentration of 3.13 mmol/cm^3 at a depth of 150 cm (ON-2) after 9.6 days.
- Further dispersion results in a maximum concentration of only 2.2 mmol/cm^3 after 19.7 days at the lower boundary (ON-3).

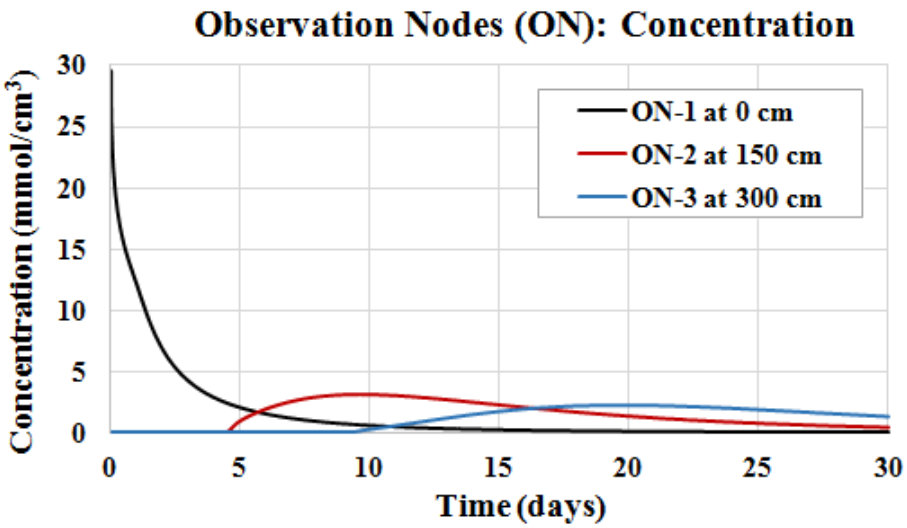

Figure 5c.1. Solute concentrations versus time at selected observation points.

Profile Information

Figure 5c.2 shows how the initial solute mass travels down the profile with the peak concentration decreasing down the profile due to dispersion.

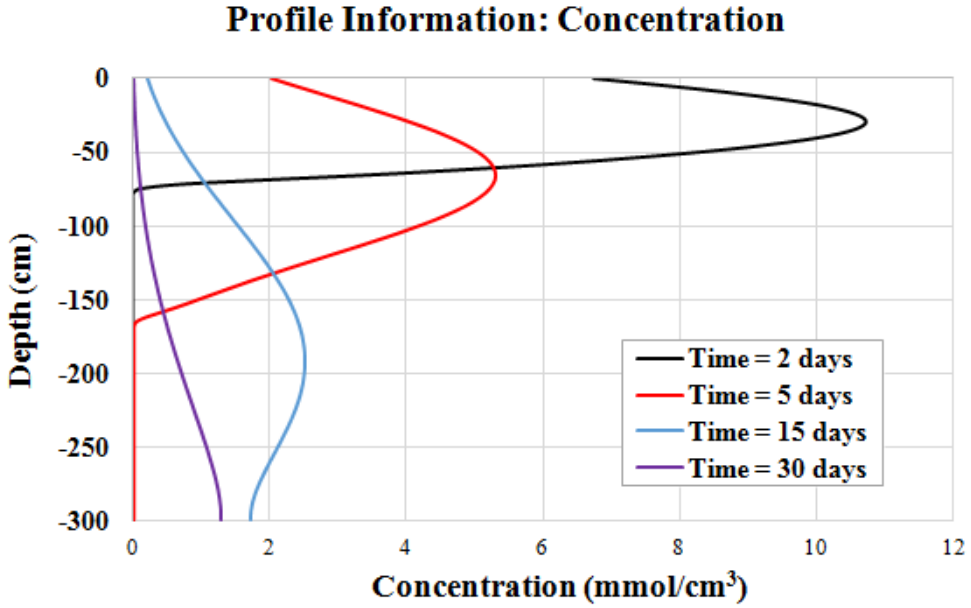

Figure 5c.2. Concentration profiles at selected times.

Solute Fluxes

Figure 5c.3 shows the bottom solute flux, which peaks just after about 20 days, which almost coincides with the time when the solute concentration peaks at the same location (see Figure 5c. 5c.1, ON-3 at 300 cm depth). Recall that solute fluxes are positive when entering the transport domain and negative when leaving the transport domain.

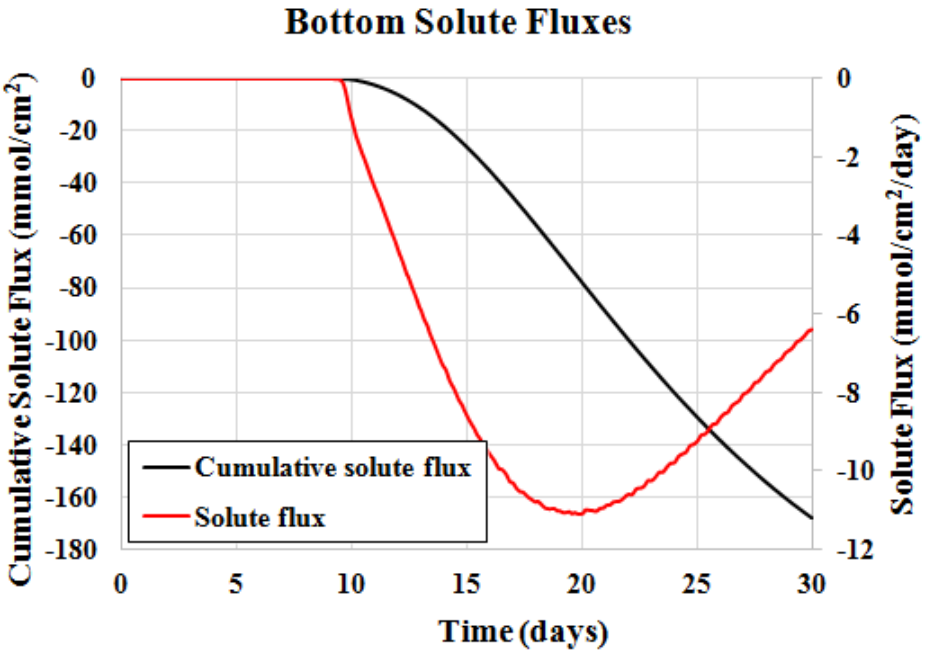

Figure 5c.3. Actual and cumulative bottom solute fluxes versus time.

Example 5d: Basic Solute Transport: The Effects of Solute Dispersion

Example Description and Objectives

The objective of Example 5d is to demonstrate the effect of solute dispersion (through the use of different values of the dispersivity) on solute transport. By reducing the dispersivity, advective transport becomes more dominant, leading to sharper concentration fronts. Example 5d is identical to Example 5c except that it uses a much smaller dispersivity parameter (D_L = 2 cm) compared to the previous example (D_L = 30 cm).

Example 5d thus simulates water flow and solute transport through a 300-cm deep uniform soil profile with an initial pressure head of -100 cm. The soil profile has a solute mass stored within the top 30 cm (concentration = 30 mmol/cm^3). Solute-free water is introduced through the upper 'Constant Flux' boundary' during the entire 30-day simulation. Water drains through the bottom 'Free Drainage' boundary.

Pre-Processing

This example will be created by copying and renaming Example 5c and then modifying it.

Project Manager

- Select the *Projects* Tab
- Select *Example 5c*
- Button "Copy"
- New Name: Example 5d
- Description: Basic Solute Transport - Showing the effects of dispersivity
- *Button* "OK"
- Select *Example 5d*
- Button "Open"

Main Processes

- Heading: Show the effect of dispersivity
- *Button* "OK"

Since the problem is identical to Example 5c (except for the dispersivity value), we can skip all input dialog windows except for the **Solute Transport Parameters** dialog window.

Solute Transport - Transport Parameters

- Disp. = 2 (cm)
- *Button* "OK"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D, or a Toolbar button  .
- The dialog window appears and asks "**Do you want to save the input data before executing HYDRUS-1D?"**.

- *Button* “Yes” (the input data need to be saved before the computational module can be run).
- The dialog window appears and warns "**All existing output files will be deleted. Continue?"**. When output files exist, the program issues a warning that they will be deleted if the computational module is run.
- *Button* “Yes”

Post-Processing

Observation Points

Compare Figure 5d.1 (lower dispersion) to Figure 5c.1 (higher dispersion):

- The peak concentrations are higher.
- The peak concentrations appear at a later time.
- Solute advances in a more advective manner (i.e., closer to piston flow).

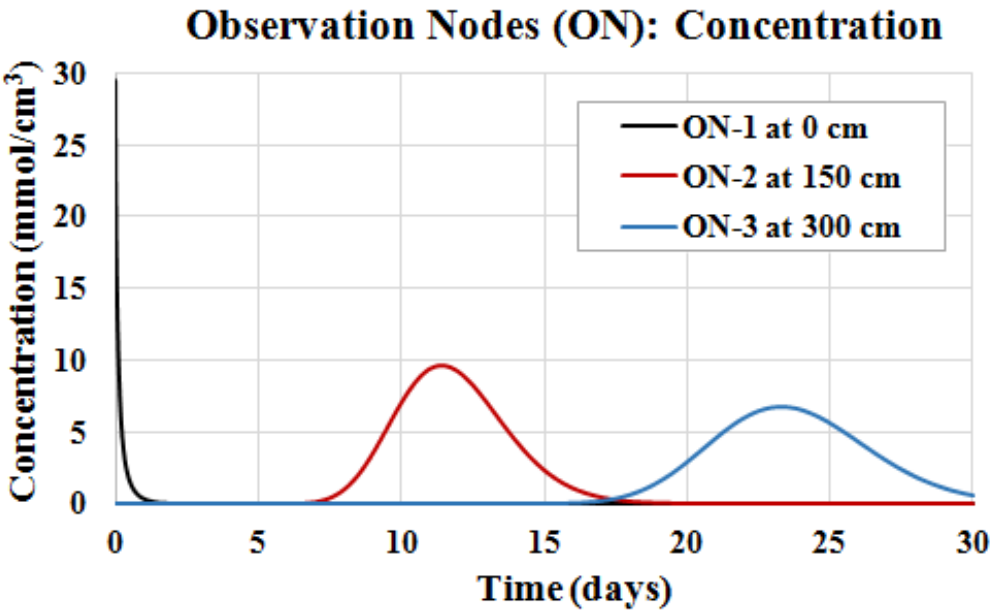

Figure 5d.1. Solute concentration versus time at selected observation points

Profile Information

Compare Figure 5d.2 (lower dispersion) to Figure 5c.2 (higher dispersion):

- Solute moves as a narrower bulge, while having a higher peak concentration.
- Solute breaks through at the lower boundary at a later time.

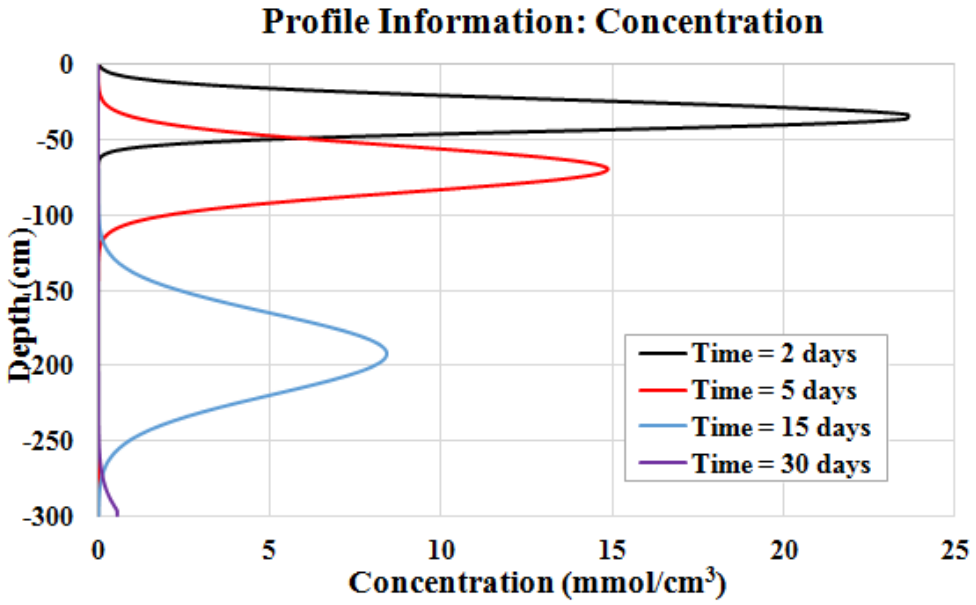

Figure 5d.2. Profile concentrations at selected times

Solute Fluxes

Compare Figure 5d.3 (lower dispersion) to Figure 5c.3 (higher dispersion):

- The solute flux peak is higher.
- Solute breaks through the lower boundary at a later time.

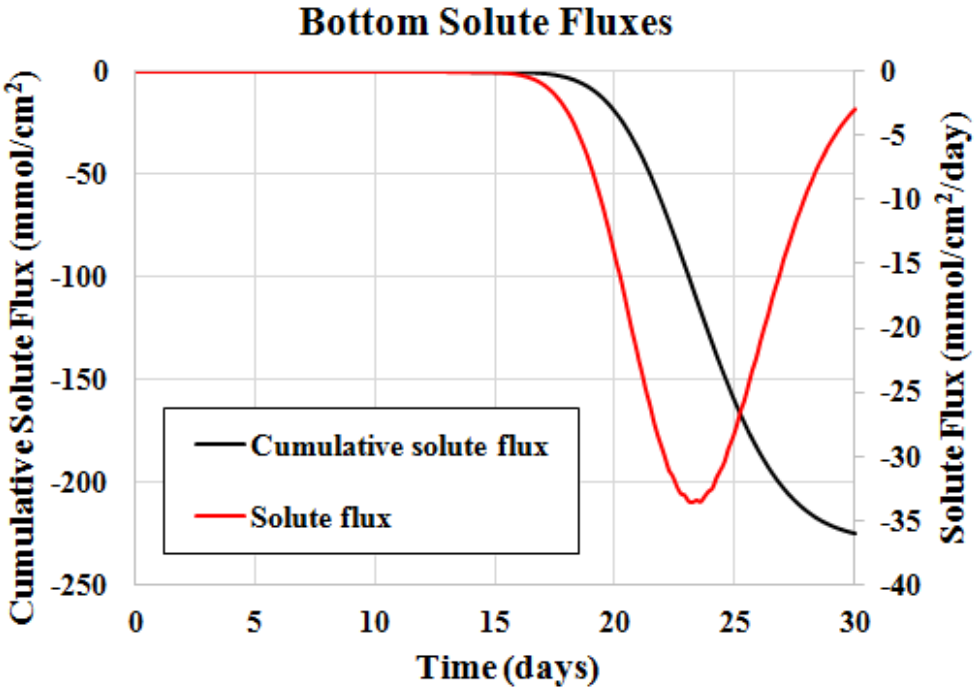

Figure 5d.3. Bottom solute fluxes versus time

Run Time Information

Referring to Figure 5d.4:

- Note a much higher Peclet number in Example 5d (less dispersion) compared to Example 5c (high dispersion). Higher Peclet numbers indicate a higher ratio of advective transport to dispersive transport.
- The Peclet number reached a value of 2 during the simulation. We recommend that when Peclet numbers close to two or higher are obtained, the mass balance should be checked (in this case, the relative error in the solute mass balance is only 0.15%). Note that for much lower dispersivities (and correspondingly higher Peclet numbers), the current time and space weighting schemes may not be appropriate and may lead to unacceptable mass balance errors. When this happens you may need to implement a finer spatial discretization or use various stabilizing options (e.g., using upstream weighting or a stability criterion). We refer to the Chapter 8.4.5 of the HYDRUS-1D Technical Manual for details.

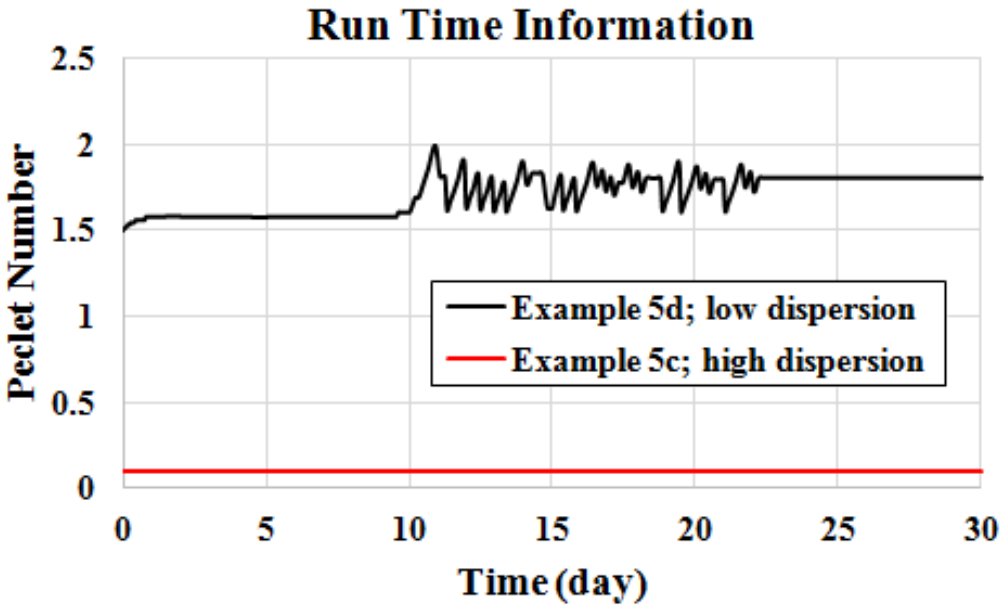

Figure 5d.4. Stability Criteria versus time

Example 5e: Basic Solute Transport: The Effects of Diffusion

Example Description and Objectives

The objective of Example 5e is to demonstrate the effect of diffusion on solute transport. Example 5e simulates steady-state water flow and solute transport through a vertical saturated 100-cm uniform soil profile. The pressure head is equal to zero everywhere in the soil column. The same pressure head is also imposed on the two 'Constant Pressure Head' boundaries (i.e., the upper and lower boundaries). As a result, flow occurs only due to gravity and the fluid flux is equal to the saturated hydraulic conductivity. Water having a unit solute concentration is introduced through the upper 'Constant Pressure Head' during the entire 1,000-day simulation. Because the soil profile is fully saturated, the soil hydraulic parameters (except for the saturated water content and the saturated hydraulic conductivity) are irrelevant. The saturated hydraulic conductivity K_s has a very low value of 0.001 cm/d, under which conditions the contribution from molecular diffusion to solute transport becomes important. Two simulations are carried out using diffusion coefficients of 0.10 cm^2/day (marked as Low Diffusion) and 2.0 cm^2/day (marked as Typical Diffusion), the latter being a good rule-of-thumb value for the molecular diffusion coefficient in water. Note that we set the dispersivity equal to zero and disabled the tortuosity factor so that the soil diffusion coefficient is equal to the specified molecular diffusion coefficient. This example demonstrates the critical role of solute diffusion when flow rates are extremely low.

Pre-Processing

Project Manager

- Select *Projects* Tab
- Button “New”
- Name: Example 5e1
- Description: Basic Solute Transport - Typical Diffusion
- *Button* “OK”

Main Processes

- Heading: Show the effect of diffusion
- Uncheck "Water Flow"
  (When the "Water Flow" option is unchecked, the initial pressure head distribution is kept constant during the simulation. For example, when the pressure head is kept constant and equal to zero, the gravitational flow will result in a steady-state water flux equal to the saturated hydraulic conductivity.)
- Check “Solute Transport”
- *Button* “Next”

Geometry Information

- Keep default values
- Depth of Soil Profile (cm): 100 cm
- *Button* “Next”

Time Information

Time Discretization:
- Final Time (day): 1000
- *Button* “Next”

Print Information
- Keep default values
- Number of Print Times: 5
- *Button* “Select Print Times”
- *Button* “OK”
- *Button* “Next”

Water Flow – Iteration Criteria
- Keep default values
- Click *Button* “Next”

Water Flow – Soil Hydraulic Model
- Keep default values (Single Porosity Models, van Genuchten – Mualem)
- Click *Button* “Next”

Water Flow – Soil Hydraulic Parameters
- Click *Button* “Next”
- Qr=0, Qs=0.4, Alpha=0.01 n=1., Ks=0.001 cm/d, l=0.5
  (note that under saturated conditions, only the saturated water content, Qs, and the saturated hydraulic conductivity, Ks, are relevant. The values of other parameters are not important.)
- *Button* “Next”

Water Flow – Boundary Conditions
- Upper Boundary Condition: Constant Pressure Head
- Lower Boundary Condition: Constant Pressure Head
- Initial Condition: In Pressure Heads
  (This setup ensures that the pressure head throughout the soil column and during the entire simulation will remain constant and equal to zero. As a result, only the gravitational flow will occur.)
- *Button* “Next”

Solute Transport
- Keep default values
- Uncheck “Use Tortuosity Factor” (to keep the soil diffusion coefficient equal to the molecular diffusion coefficient in water)
- Pulse duration (day): 1000
- *Button* “Next”

Solute Transport Parameters
- Disp. = 2 (cm)
- Diffus. W. = 2 (cm^2/day) [or 2.3×10^{-9} m^2/s, a Typical Diffusion transport simulation]
- *Button* “Next”

Solute Transport and Reaction Parameters

- Keep default values
- *Button* “Next”

Solute Transport Boundary Conditions

- Sol. No. 1 Bound. Cond. = 1
- *Button* “Next”

HYDRUS-1D guide

- Do you want to run PROFILE application?
- *Button* “Yes”
- Do you want to save data before running Graphical Profile Editor?
- *Button* “Yes”
- All existing output files will be deleted. Continue?
- *Button* “Yes”

Soil Profile – Graphical Editor

- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar** 
- *Button* (left side) “Edit Condition”: select with the Mouse the entire domain, left click, specify 'Pressure Head Distribution': Top value = 0, Bottom value = 0, and unchecked "Use top value for both".
- *Button* “OK”
- **Menu**: Conditions->Observation Nodes or **Toolbar** 
- *Button* (left side) “Insert”: select nodes at 50 and 100 cm (right-click to end the command)
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* “Next”

Execute HYDRUS-1D

- **Menu**: Calculation->Execute or a **Toolbar** button  .

Rerun the example with lower diffusion coefficient:

Project Manager

- Select *Projects* Tab
- Select Example 5e1
- Copy
- New Name: Example 5a2
- Description: Basic Solute Transport - Low diffusion
- Select Example 5e2
- *Button* “OK”

Solute Transport Parameters

- Diffus. W. = 0.1 (cm^2/day) [or 1.16×10^{-10} m^2/s, [a Low Diffusion simulation]
- *Button* “Next”

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

Referring to Figure 5e.1:

- The extremely low flow rate (0.001 cm/d) significantly hinders solute transport dominated by the diffusion process. The low flow rate in this example is due to the very low K_s and having a zero pressure head gradient.
- For the case of low diffusion (Diffusion coefficient = 0.1 cm^2/day), breakthrough curves at selected observation nodes are not shown because the solute front had not reached the selected nodes within the simulation period.
- Obviously, having a high diffusion coefficient significantly enhances solute transport since diffusion is then the dominant process at such low flow rates.
- Increasing the dispersivity has a very marginal impact on solute breakthrough at such low flow rates. Conversely, when flow rates are high and solute transport is dominated by dispersion processes [e.g., Example 5d], changing the diffusion coefficient hardly has any impact on solute breakthrough.

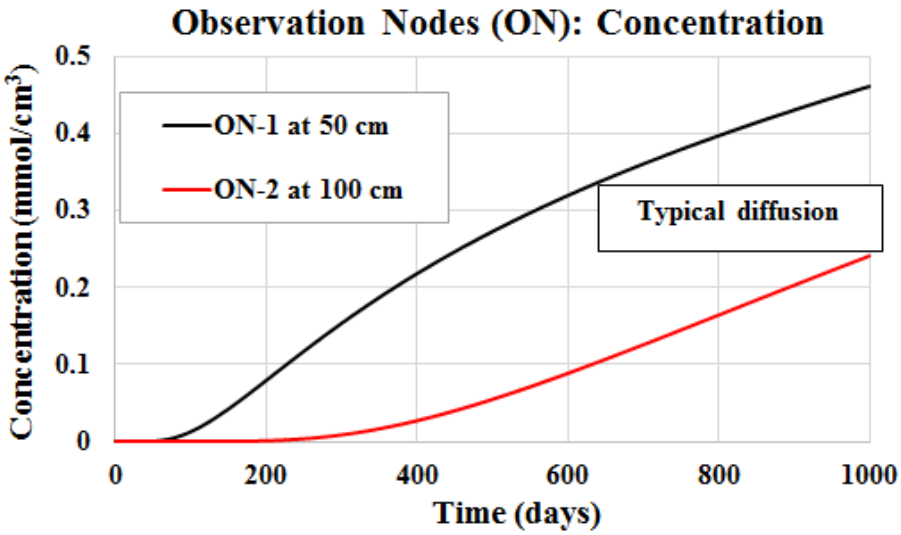

Figure 5e.1. Solute concentrations versus time at selected observation points.

Profile Information

Referring to Figure 5e.2:

- For the case of low diffusion (red lines), the solute concentration profiles show that the solute front had not yet reached a depth of 50 cm (the location of ON-1).
- A higher diffusion coefficient significantly enhanced solute breakthrough, albeit still during very long timeframes.

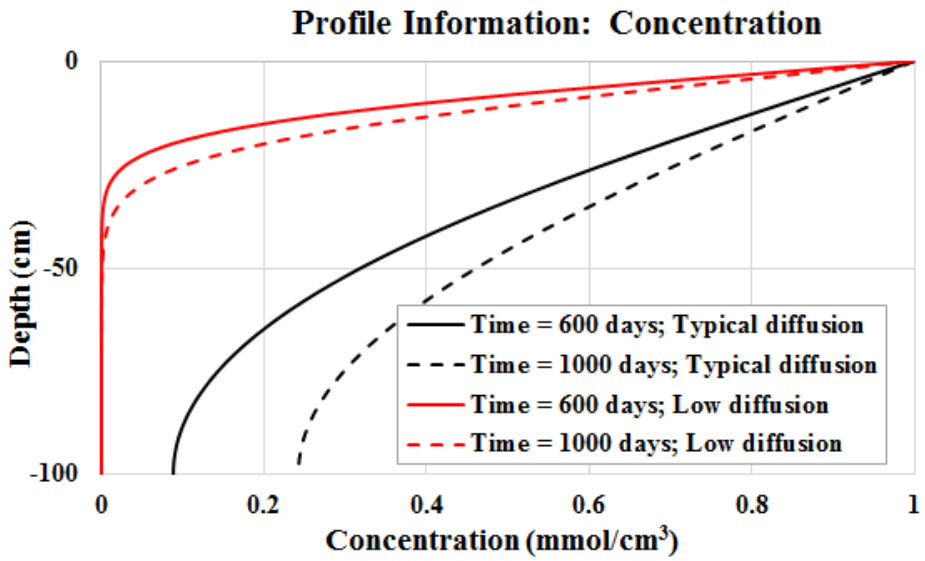

Figure 5e.2. Concentration profiles at selected times for low (red lines) and high (black lines) diffusion.

Solute Fluxes

Referring to Figure 5e.3:

- The solute mass introduced at the upper constant pressure head boundary is extremely low due to the very low flow rate.
- A higher diffusion rate leads to more solute mass entering the constant pressure head boundary where the solute is introduced.
- The cumulative bottom flux is not shown here due to its negligibly small value (only 0.038 mmol/cm^2 after 1000 days for the high diffusion case).

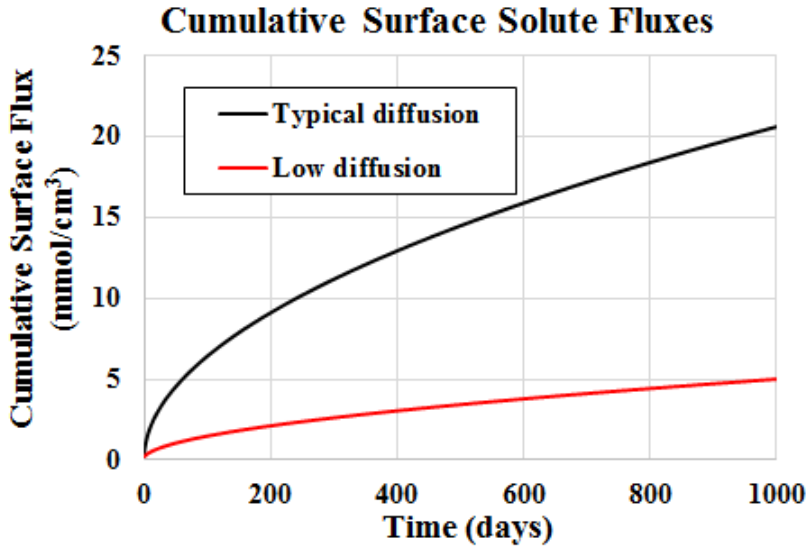

Figure 5e.3. Surface solute fluxes versus time for low (a red line) and high (a black line) diffusion.

Example 6a: Advanced Solute Transport: Equilibrium (instantaneous) Linear Sorption

Example Description and Objectives

Example 6a simulates flow and transport through an initially solute-free 300-cm deep uniform, fully saturated soil profile (having an initial pressure head of 0 cm). Water drains through the bottom 'Free Drainage' boundary. Water having a unit solute concentration is introduced through the upper 'Constant Pressure Head' boundary' during the entire 20-day simulation. Solute sorption onto the soil solid phase is introduced by considering linear equilibrium sorption, which is typically represented mathematically by the distribution coefficient (or the solid-liquid partitioning coefficient), K_d (Figure 6.a.1). Applying the K_d concept results in solutes being instantaneously sorbed to the solid phase, and in solute retardation that is described by the retardation factor R defined as:

$$R = 1 + \frac{\rho K_d}{\theta} \tag{6a.1}$$

where K_d (L/kg = cm^3/g) is an empirical distribution factor of the linear sorption isotherm that relates S (the sorbed concentration, i.e., solutes sorbed to soil particles, g solute/g soil) to C (the concentration in the liquid pore space, g solute/cm^3), θ is the water content (equal to porosity at full saturation, cm^3/cm^3) and ρ is the bulk density (g/cm^3).

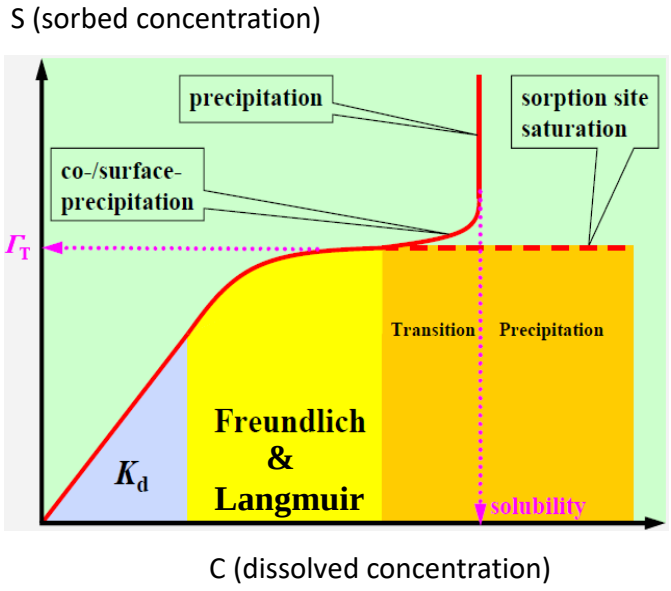

Figure 6a.1. General sorption isotherm representation, showing differences between linear (indicated as 'K_d' region) and non-linear sorption (indicated as 'Freundlich' region), a transition period left of the precipitation threshold, and solute precipitation (indicated as 'precipitation' region). The vertical axis (S) and the horizontal axis (C) are, respectively, the sorbed concentration (on solid phases) and the dissolved concentration (in the liquid phase). (Source: Wang et al., 2009).

Substituting K_d = 0.267 (cm^3/g), θ=0.4 (cm^3/cm^3), and ρ = 1.5 (g/cm^3) results in an R value of 2.0 for the present example. The retardation factor (R, dimensionless) represents the relative rate of fluid flow to the transport rate of a reactive sorbing solute (Freeze and Cherry, 1979) or:

$$R = \frac{v}{v_r} \tag{6a.2}$$

where v is fluid flow rate, v_r is the transport rate for the center of mass of the reactive solute. The retardation factor is equal to 1 for non-reactive (non-sorbing) solutes travelling in a medium where the entire pore space is effective in transporting the fluid (effective porosity=total porosity).

Example 6a demonstrates the effect of retardation when a solute is sorbed onto the soil solid phase. This process is modeled here using a simple linear model (termed a linear isotherm). The effect of retardation is demonstrated by comparing the results from two nearly identical simulations: one having R = 1 (no sorption) and the other having R = 2 (with sorption). This project will show the effect of retardation on solute breakthrough from the soil profile (or from a laboratory column). Since HYDRUS-1D does not report sorbed solute masses for the equilibrium model, the mass balance information will be used to demonstrate how this term can be calculated across the entire profile.

Pre-Processing

We create 'Example 6a1' by copying and modifying 'Example 5b' using the Project Manager.

Project Manager
- Select *Projects* Tab
- Select *Example 5b*
- Click *Button* “Copy”
- Type New Name: Example 6a1
- Type Description: Advance Solute Transport - Retardation
- Click *Button* “OK”
- Select *Example 6a1*
- Click *Button* “Open”

Main Processes
- Heading: Simulate the Effects of Retardation
- Uncheck "Water Flow" (while in Example 5b transient water flow was considered, in Example 6a1 water flow is steady-state)
- Click *Button* “OK”

Water Flow – Soil Hydraulic Parameters
- Soil Catalogue: Loam
- Qs = 0.4 [saturated water content; the value used to get round numbers in the mass balance]
- Ks = 20 [saturated hydraulic conductivity; the value used to get round numbers in the mass balance]
- *Button* “OK”

Solute Transport - General Information

- Leave default values
- Pulse duration (day): 20 [Located in the bottom right corner; to obtain a continuous solute application throughout the entire simulation period of 20 days]
- *Button* "Next"

Solute Transport - Transport Parameters

- Bulk. D. = 1.5 (g/cm^3)
- Disp. = 2 (cm)
- *Button* "Next"

Solute Transport - Reaction Parameters

- Kd = 0.267 (cm^3/g, this will invoke retardation)
- *Button* "OK"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Observation Nodes or **Toolbar** 
- *Button* (left side) "Delete": select the top node at 0 cm to delete this observation node (right-click to end the command)
- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar** 
- *Button* (left side) "Edit Condition": select with the Mouse the entire profile and specify the Pressure Head of 0 cm.
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Rerun the example without retardation:

Project Manager

- Select *Projects* Tab
- Select Example 6a1
- Copy
- New Name: Example 6a2
- Description: Advance Solute Transport - No Retardation
- Select Example 6a2
- *Button* "OK"

Solute Transport - Reaction Parameters

- Kd = 0 (without retardation)
- *Button* "OK"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

- Figures 6a.2 and 6a.3 show that retardation delays solute breakthrough by a factor of two (R = 1+0.267×1.5/0.4 = 2) since a fraction of the solute is sorbed to the soil particles.
- Figures 6a.2 and 6a.3 show that a steady-state concentration of unity (equal to the concentration applied at the inlet constant pressure head boundary) has been achieved in the profile.

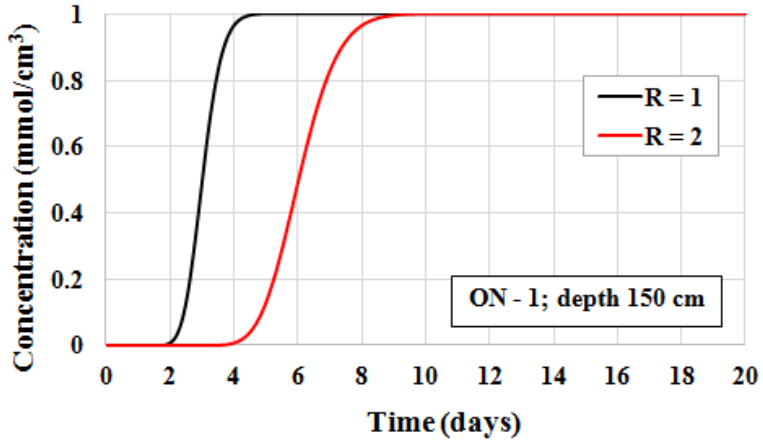

Figure 6a.2. Liquid phase solute concentrations versus time with (R=2) and without (R=1) sorption at ON-1.

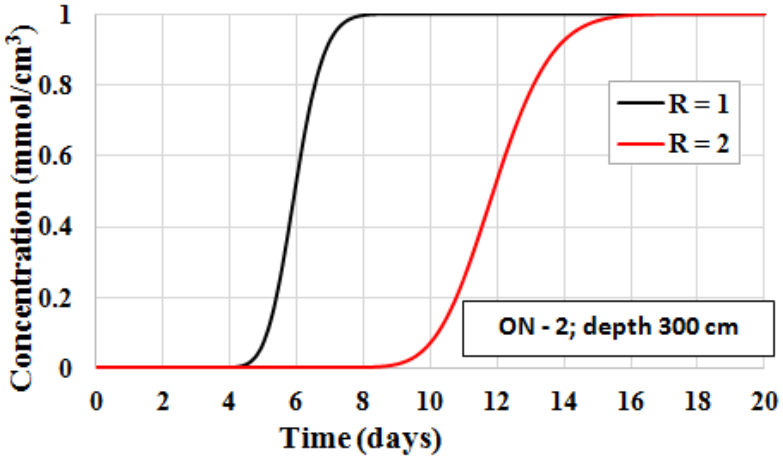

Figure 6a.3. Liquid phase solute concentrations versus time with (R=2) and without (R=1) sorption at ON-2.

- Figure 6a.4 displays the concept of dimensionless time (Skaggs and Leij, 2002). The use of dimensionless time is useful since it eliminates the effects of travel

distance and flow velocity, which are specific to any one experiment. Dimensionless time as used here is also known as the number of pore volumes and represents the cumulative outflow volume from a soil profile or laboratory column, divided by the volume of fluid in the system. Travel time t is the ratio of distance to average pore-water velocity (L/v). To obtain dimensionless time, T, we multiply time t by this ratio (v/L) to get:

$$T = \frac{vt}{L} \tag{6a.3}$$

Multiplying Eq. 6a.3 by A/A, where A is the cross-sectional area of the system being considered, gives

$$T = \frac{vtA}{LA} = \frac{QA}{LA} = \frac{V_{eluted}}{V_{available}} \tag{6a.4}$$

where T (number of pore volumes) represents how many times the fluid content of the column has been displaced by the influent fluid. In this example, T is calculated as follows:

$$T = \frac{20t}{300 * 0.40} \tag{6a.5}$$

where the flux is 20 cm/day, the column length is 300 cm, and the water content is 0.40. Figure 6a.4 shows that the center of solute mass breaks through after about 1 pore volume (when nonequilibrium processes are present solute does not break through at one pore volume), and that sorption delays it by another pore volume. In fact, one can show that the number of displaced pore volumes is mathematically equal to R (in reality the area above the curves in Fig. 6a.4).

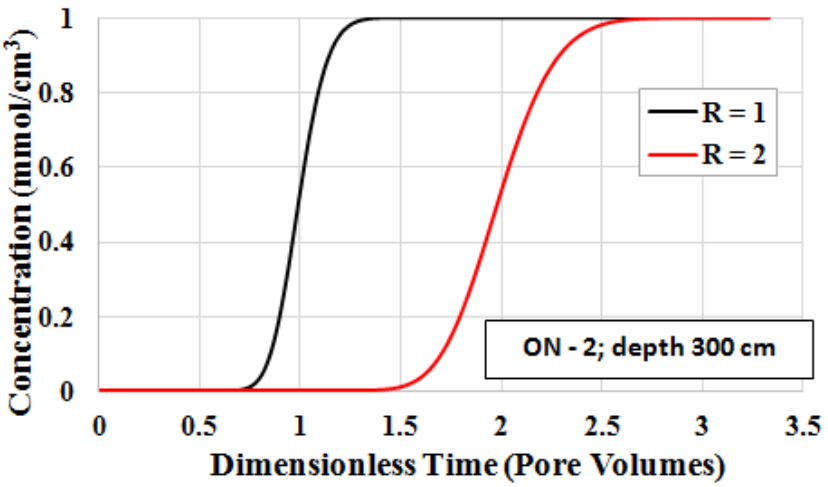

Figure 6a.4. Liquid phase solute concentrations versus dimensionless time with (R=2) and without (R=1) retardation at ON-2.

Profile Information

Figure 6a.5 shows solute profile concentrations after 4 and 8 days. Note that identical profiles are obtained when doubling the residence time and doubling the retardation factor.

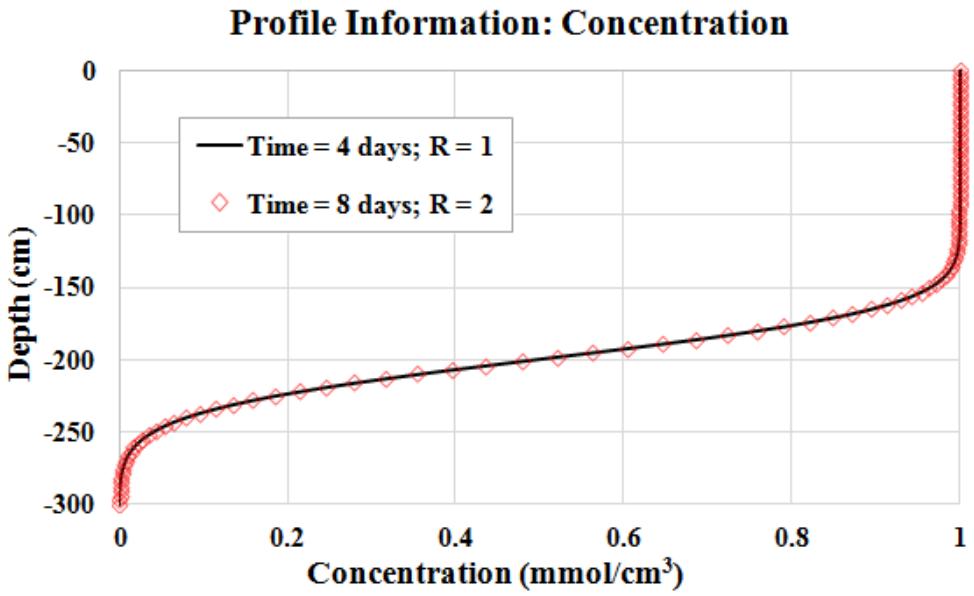

Figure 6a.5. Liquid phase solute concentration profiles with (R=2) and without (R=1) retardation at different times.

Solute Fluxes

- Figure 6a.6 shows cumulative solute fluxes at the surface (inlet) and bottom (outlet) boundaries. When solute retardation is active (R=2), solutes become sorbed onto the solid phase and hence less solute mass (since some solute mass is stored at the sorption sites) is observed at the bottom boundary compared to the case when retardation is absent. Note that the breakthrough at the end of the column starts at about 5 and 10 days for R equal to 1 and 2, respectively, reflecting the retardation factors ratio of 2.

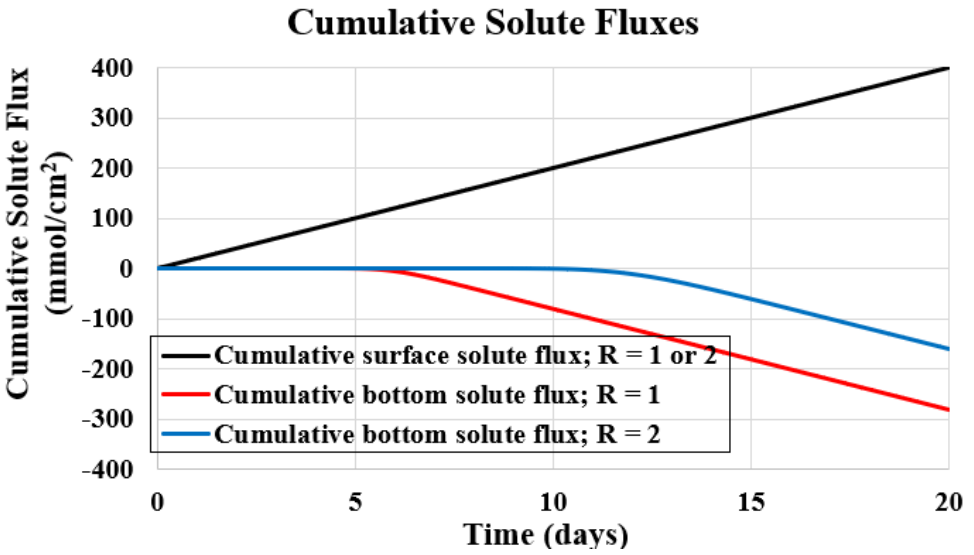

Figure 6a.6. Cumulative surface and bottom solute fluxes versus time with (R=2) and without (R=1) retardation.

Mass Balance Information

HYDRUS-1D does not explicitly report sorbed concentrations (S) since they can be easily calculated from the adsorption isotherm and the liquid phase concentrations (C), i.e., $S=K_d \times C$. The information reported in the mass balance file can be used to derive the sorbed mass. Note that the calculations below use data from the entire profile (since only one subregion was used) and hence produce correct results only when a steady-state concentration has been reached [in this case, cMean = 1 mmol/cm^3].

The mass balance information refers to the following:

Length: Depth of the soil profile
W-volume: Total volume of soil water
In-flow: The sum of fluxes flowing into and out of the soil profile (or subregion)
h Mean: The average pressure head in the soil profile
ConcVol: The total solute mass in the profile (in the liquid phase and sorbed equilibrium phase)
cMean: The mean concentration in the liquid phase
Top Flux: The flux into the soil profile
Bot Flux: The flux out of the soil profile
WatBalT: The total water balance error in the soil profile
WatBalR: The relative water balance error in %

Table 6a.1 compares mass balance information at the end of the simulation (day 20). Note that the total combined solute mass in the liquid and sorbed phases (ConcVol) is 240 mmol/cm^2 when R=2 compared to 120 mmol/cm^2 when R=1.

Table 6a.1. Mass balance information for Time = 20 days with (R=2) and without (R=1) retardation.

		R = 2	R = 1
Length	[L]	300	300
W-volume	[L]	120	120
In-flow	[cm/day]	0	0
H Mean	[L]	0	0
ConcVol	[mmol/cm^2]	240	120
cMean	[mmol/cm^3]	1.00	1.00
Top Flux	[cm/day]	-20	
Bot Flux	[cm/day]	-20	
WatBalT	[cm]	0	
WatBalR	[%]	0	
CncBalT	[mmol]	1.20	0.6
CncBalR	[%]	0.214	0.088

By definition, K_d is an empirical distribution factor of the linear sorption isotherm that relates S (sorbed concentration) to C (resident concentration):

$$K_d = \frac{S}{C} \tag{6a.7}$$

We substitute Equation 6a.7 into Equation 6a.1 and obtain:

$$R = 1 + \frac{S\rho}{C\theta} \tag{6a.8}$$

where $C\theta$ is the mass of solute in the liquid phase and $S\rho$ is the mass of sorbed solute per unit soil volume.

Referring to Table 6a.1, for the case when R=2:

ConcVol = 240 mmol/cm^2
W-volume = 120 cm^3
cMean = 1 mmol/cm^3 (this calculation works well here as the profile has reached a steady state)

Mass in the liquid phase = $C\theta$ = 1 x 120 = 120 mmol

$S\rho$ [sorbed mass] = ConcVol [total mass] – $C\theta$ [mass in liquid phase] = 240 – 120 = 120 mmol

$R = 1 + \frac{S\rho}{C\theta} = 1 + \frac{120}{120} = 2$ [Implemented in this example]

Example 6b: Advanced Solute Transport: Non-Linear Equilibrium Non-Linear Sorption

Example Description and Objectives

Example 6b simulates water flow and solute transport through a 100-cm horizontal uniform saturated soil profile having a 10% pressure head gradient imposed across two Constant Pressure Head Boundaries. Water having a 10 mmol/cm^3 solute concentration is introduced to the initially solute-free soil profile through the upper 'Constant Pressure Head' boundary during the entire 50-day simulation. Sorption is modeled using a non-linear Freundlich-Langmuir isotherm given by

$$S = \frac{K_d C^{\beta}}{1+\eta C^{\beta}} \tag{6b.1}$$

where S is the sorbed concentration (solutes sorbed onto the solid phase), C is the liquid phase resident concentration, and K_d, β and η are empirical or quasi-empirical constants. The units for K_d are ($L^{3\beta}$ $M^{-\beta}$) and those for η are (L^3M^{-1}). When β=1, Eq. (6b.1) becomes a Langmuir isotherm, when η=0, the equation becomes a Freundlich isotherm, and when both β=1 and η=0 the equation reduces to a linear sorption isotherm (Eq. 6a.7). The Freundlich and Langmuir isotherms are shown in Figure 6b.1 for different values of the parameters β and η. For nonzero (positive) values, the Langmuir coefficient η leads to an upper limit (given by K_d/η) that sorbed concentrations cannot exceed, while the Freundlich exponent β dictates how quickly this saturation limit is achieved. We use this example to demonstrate how solute transport is affected by with nonlinear sorption.

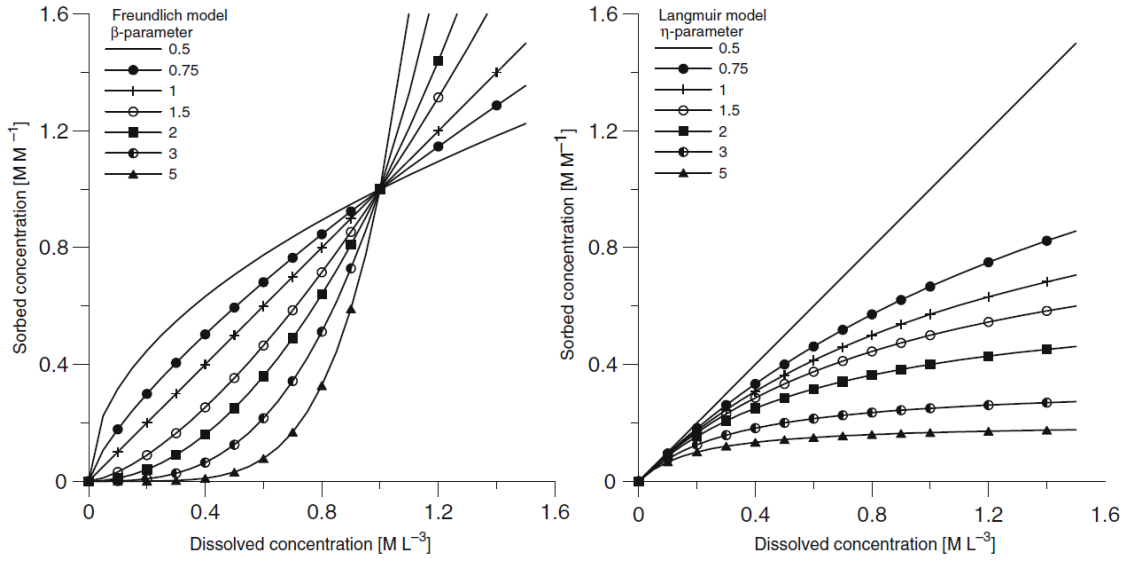

Figure 6b.1. Plots of the Freundlich adsorption isotherm given by Eq. (6b.1, η= 0), with K_d = 1 and β defined in the caption (left), and the Langmuir adsorption isotherm given by Eq. (6b.1, β=1), with K_d = 1 and η defined in the caption (right) (source: Mallants et al., 2011)

Pre-Processing

Project Manager

- Select *Projects* Tab
- Button “New”
- Name: Example 6b
- Description: Advance Solute Transport - Equilibrium nonlinear sorption
- *Button* “OK”
- Select *Example 6b*
- Button “Open”

Main Processes

- Heading: Solute transport with non-linear sorption
- Uncheck "Water Flow"
  (When the "Water Flow" option is unchecked, the initial pressure head distribution is kept constant during the simulation. For example, when the pressure head is kept constant and equal to zero, gravitational flow in the soil profile will result in a steady-state flux equal to the saturated hydraulic conductivity.)
- Check “Solute Transport”
- *Button* “Next”

Geometry Information

- Decline from Vertical Axis: 0 (horizontal flow and transport)
- Depth of Soil Profile (cm): 100 cm
- *Button* “Next”

Time Information

Time Discretization:

- Final Time (day): 50
- *Button* “Next”

Print Information

- Print Options: Leave as Default
- Number of Print Times: 12
- *Button* “Select Print Times”
- *Button* “Default”
- *Button* “OK”
- *Button* “Next”

Iteration Criteria

- Leave as Default
- *Button* “Next”

Water Flow – Soil Hydraulic Model

- Leave as Default
- *Button* “Next”

Water Flow – Soil Hydraulic Parameters

- Soil Catalogue: Loam
- Qs = 0.4 (to get round numbers in the mass balance)
- Ks = 20 (to get round numbers in the mass balance)
- *Button* “Next”

Water Flow – Boundary Conditions

- Upper Boundary Condition: Constant Pressure Head
- Lower Boundary Condition: Constant Pressure Head
- *Button* “Next”

Solute Transport

- Leave as Default
- Pulse duration (day) 50
  Iteration Criteria: (Need to be specified for nonlinear solute transport problems. Nonlinear sorption causes the problem to be nonlinear.)
- Absolute Concentration Tolerance = 0.001
- Relative Concentration Tolerance = 0.001
- Maximum Number of Iterations = 20
- *Button* “Next”

Solute Transport Parameters

- Bulk. D. = 1.5 (g/cm^3)
- Disp. = 10 (cm)
- *Button* “Next”

Solute Transport and Reaction Parameters – Solute 1

- K_d = 0.267 ($cm^{3\times2}/g^2$), because Beta = 2)
- Nu = 0.1 (cm^3/g)
- Beta = 2.0 (-)
- *Button* “Next”

Solute Transport Boundary Conditions

- Sol. No. 1 Bound. Cond. = 10 $mmol/cm^3$
- *Button* “Next”

Soil Profile – Graphical Editor

- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar** 
- *Button* (left side) “Edit Condition”: select with the Mouse the entire domain, left click
- Pressure Head Distribution: Top value = 10 (this in fact a left-side value for the horizontal soil profile), Bottom value = 0 (a right-side value), uncheck "Use top value for both"
- *Button* “OK”
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* “Next”

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

Figure 6b.2 shows breakthrough curves of the liquid and sorbed concentrations at depths of 50 and 150 cm in the soil profile. Solute concentrations in the liquid phase approach the applied concentration of 10 mmol/cm^3 but do not quite reach it. Note that sorbed concentrations (which are not reported by HYDRUS-1D) were calculated directly from the liquid phase concentrations using the sorption isotherm (eq. 6b.1).

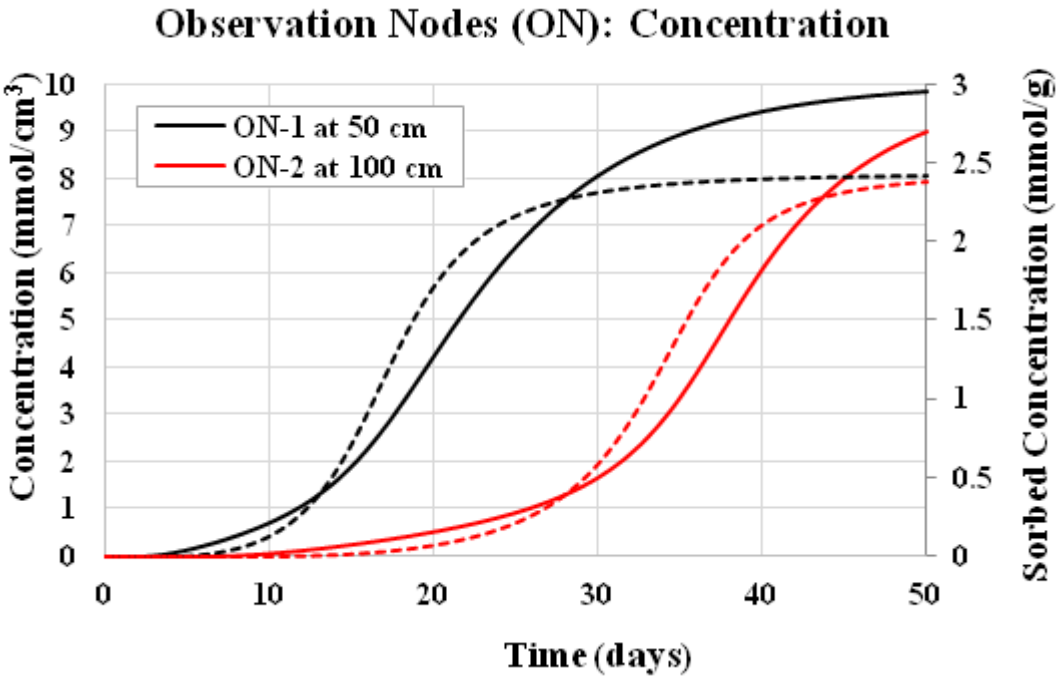

Figure 6b.2 Solute concentrations in the liquid (solid lines) and sorbed (dashed lines) phases versus time at depths of 50 and 100 cm.

Profile Information

Figure 6b.3 shows calculated solute concentration profiles at different times. They confirm that concentrations at the end of the simulation (the blue line) have not yet reached the steady state concentration of 10 mmol/cm^3.

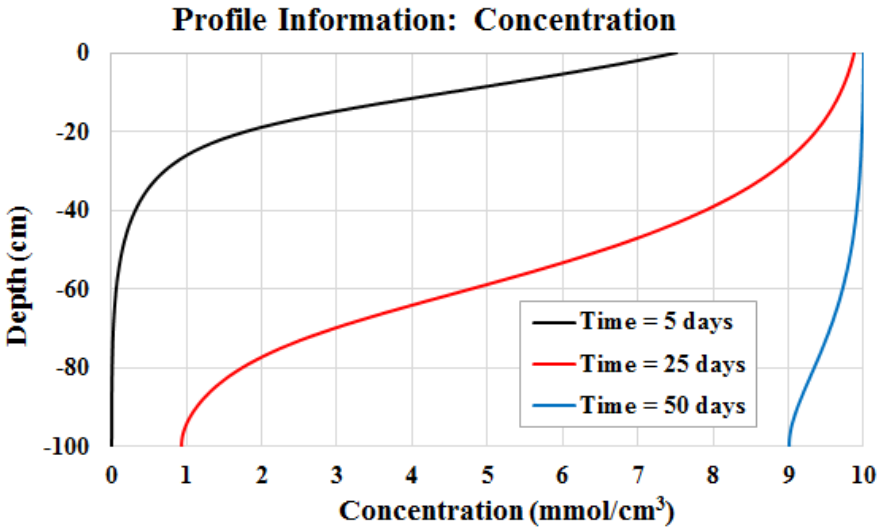

Figure 6b.3. Concentration profiles at different times.

Example 6c: Advanced Solute Transport: One-Site Chemical Nonequilibrium Sorption

Example Description and Objectives

Example 6c includes three simulations of water flow and solute transport through a 100-cm uniform saturated horizontal soil profile. Water having various solute concentrations is introduced into the initially solute-free profile through the upper (left-side) 'Constant Pressure Head' boundary during the entire simulation period. Chemical nonequilibrium is modeled using the one-site sorption model (Figure 6c.1), in which a first-order rate coefficient (Alpha) controls time-dependent (not instantaneous) solute mass transfer between the liquid and solid phases. For example, the Alpha rate constant of 0.05 d^{-1} adopted in the three simulations below means that solutes in the liquid phase are transferred to the sorption sites at a rate of approximately 5% per day. The Freundlich-Langmuir isotherm is used similarly as in Example 6b, indicating that there is an upper value for the sorbed phase concentration when an equilibrium state is reached. The one-site chemical nonequilibrium sorption equation is then given by:

$$\frac{dS}{dt} = \alpha \left(\frac{K_d C^{\beta}}{1 + \eta C^{\beta}} - S \right) \tag{6c.1}$$

where (Alpha in HYDRUS-1D) is the rate coefficient.

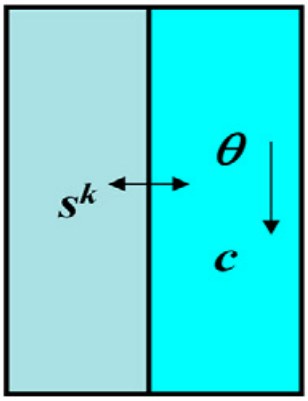

Figure 6c.1. Conceptual representation of chemical nonequilibrium one-site sorption. The parameter S^k is the kinetically sorbed solute concentration on the solid phase.

In the first two simulations (i.e., 6c1 and 6c2), pressure head gradients of 10% and 5% are imposed across the two Constant Pressure Head boundaries to demonstrate the effect of residence time on non-equilibrium sorption. Simulation times are 50 and 100 days in the two simulations, so that the total inlet solute mass is equal in both cases. The third simulation (6c3) uses a much higher inlet concentration of 1,000 mmol/cm^3 (compared to 10 mmol/cm^3 in the other two simulations), a longer simulation time of 200 days, and a 10% pressure head gradient to ensure that the saturation sorbed concentration is achieved.

This example demonstrates that time can be an important factor affecting solute mass transfer between the liquid phase and solid phases for the solute transport under

chemical nonequilibrium conditions. Since mass transfer is time-dependent, the residence time plays a crucial role since at lower flow rates the mass transfer between the liquid and solid phases becomes more effective. Since solutes are introduced into the soil profile at different rates, we will use dimensionless time to enable comparisons between simulations that have different inlet fluxes.

Pre-Processing

Project Manager

- Select *Projects* Tab
- Select *Example 6b*
- Button "Copy"
- New Name: Example 6c
- Description: Advance Solute Transport - Chemical non-equilibrium
- *Button* "OK"
- Select *Example6b*
- Button "Open"

Main Processes

- Heading: Solute transport with chemical non-equilibrium
- *Button* "Next"

Time Information

Time Discretization:

- Final Time (day): 50 (Simulation 6c1), 100 (Simulation 6c2),
  Final Time (day): 200 (Simulation 6c3)
- *Button* "OK"

Solute Transport

Non-equilibrium Solute Transport Models

- Check One-site sorption model (chemical non-equilibrium)
- Pulse duration (day): 50 (Simulation 6c1), 100 (Simulation 6c2), 200 (Simulation 6c3)
- *Button* "Next"

Solute Transport Parameters

- Frac. = 0 (all sorption sites are kinetic – as in Figure 6c.1; no equilibrium sorption)
- *Button* "Next"

Solute Transport and Reaction Parameters – Solute 1

- K_d = 0.267 ($cm^{3\times2}/g^2$) (keep the same sorption parameters)
- Nu = 0.10 (cm^3/g)
- Beta = 2.0 (-)
- Alpha = 0.05/day (need to scroll to the right of the table to find this last parameter)
- *Button* "Next"

Solute Transport Boundary Conditions

- Sol. No. 1 Bound. Cond. = 10 $mmol/cm^3$ (Simulations 6c1 and 6c2)

- Sol. No. 1 Bound. Cond. = 1000 mmol/cm^3 (Simulation 6c1)
- *Button* "Next"

Soil Profile – Graphical Editor
- **Menu**: Conditions->Initial Conditions->Pressure Head
- *Button* (left side) "Edit Condition": select with the Mouse the entire domain, then left click
- Pressure Head Distribution: Top value = 10 (for Simulations 6c1 and 6c3)
- Pressure Head Distribution: Top value = 5 (for Simulation 6c2)
  Bottom value = 0; uncheck "Use top value for both" (for all three Simulations)
- *Button* "OK"
- **Menu**: File->Save Data
- **Menu**: File->Exit

Soil Profile – Summary
- *Button* "Next"

Execute HYDRUS-1D
- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Solute Fluxes
- Dimensionless time is calculated according to Equation 6a.3 ($T=vt/L$). For simulations 6c.1 and 6c.3, the pore-water velocity (v) was equal to 5 cm/day (the pressure head gradient (0.10) times K_s (20) divided by the water content (0.4), while for simulation 6c.2, v was equal to 0.05 * 20/0.4 = 2.5 cm/day; L was 100 cm for all simulations.
- Simulation 6c1 with the higher flux of 2.0 cm/day is marked as 'Low Residence Time', whereas Simulation 6c2 with the lower flux of 1.0 cm/day is marked as 'High Residence Time'.
- Referring to Figures 6c.2: For a longer residence time, more time is available during which the time-dependent non-equilibrium solute mass transfer process occurs, resulting in a more cumulative transfer of solutes to the sorption sites.
- Figure 6c.3 shows that for the example with a long residence time, more solute mass is transferred to the sorption sites, which means that less solute mass remains in the liquid phase and hence less cumulative solute mass exits the bottom boundary at a given time compared to the simulation with the shorter residence time.

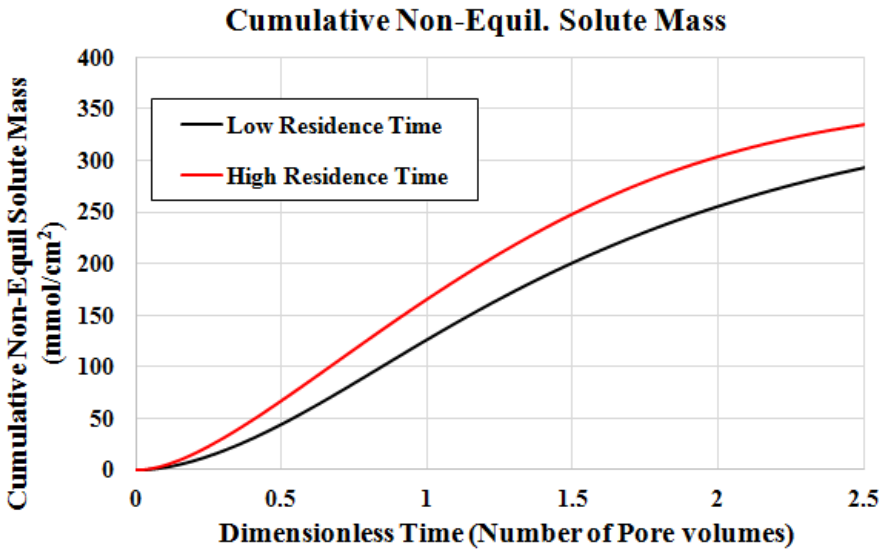

Figure 6c.2 Effect of the residence time on the non-equilibrium solute mass transfer.

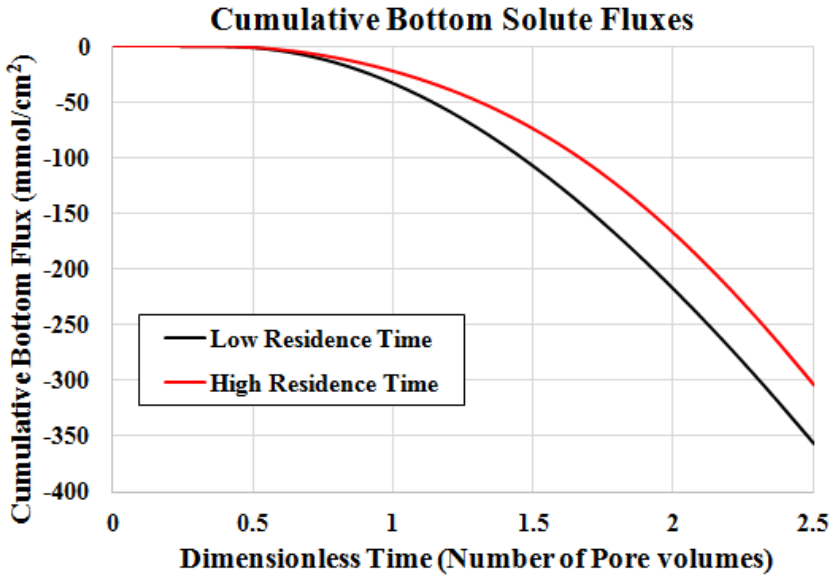

Figure 6c.3. Effect of the residence time on the cumulative bottom solute flux.

Mass Balance Information

Nonequilibrium concentrations are not explicitly reported in the 'Observation Node' file (Obs_nod.out) of HYDRUS-1D (as opposed to the HYDRUS (2D/3D) software package). However, they are reported at Print Times in the Mass Balance file (Balance.out). The same technique as adopted in Example 6b.3 is used to calculate non-equilibrium solute breakthrough at a depth of 50 cm based on the data reported for Subregion 2 at each Print Time.

- Consistent with the trend shown in Figure 6c.2, Figure 6c.1 shows a higher non-equilibrium concentration in the case of 'High Resident Time' compared to 'Low Resident Time'.
- Simulations 6c.1 and 6c.2 both did not achieve an equilibrium state, and hence the non-equilibrium concentration did not reach the saturation concentration of 2.67 mmol/cm^3 (K_d/η = 0.267/0.1 = 2.67 mmol/cm^3). Increasing the simulation time and the inlet concentration in simulation 6c.3 did achieve this goal (see the blue time series marked as 'Steady State' in Figure 6c.4).
- A practical application of modeling sorption processes is for reactive barriers installed down-gradient of a contaminated groundwater plume. One common type of reactive barrier is an interception-sorption trench filled with sorptive material that captures the groundwater contaminants. The sorptive material is then subsequently disposed of in a land fill when it can longer attract more contaminants (when it reaches the saturation concentration limit).

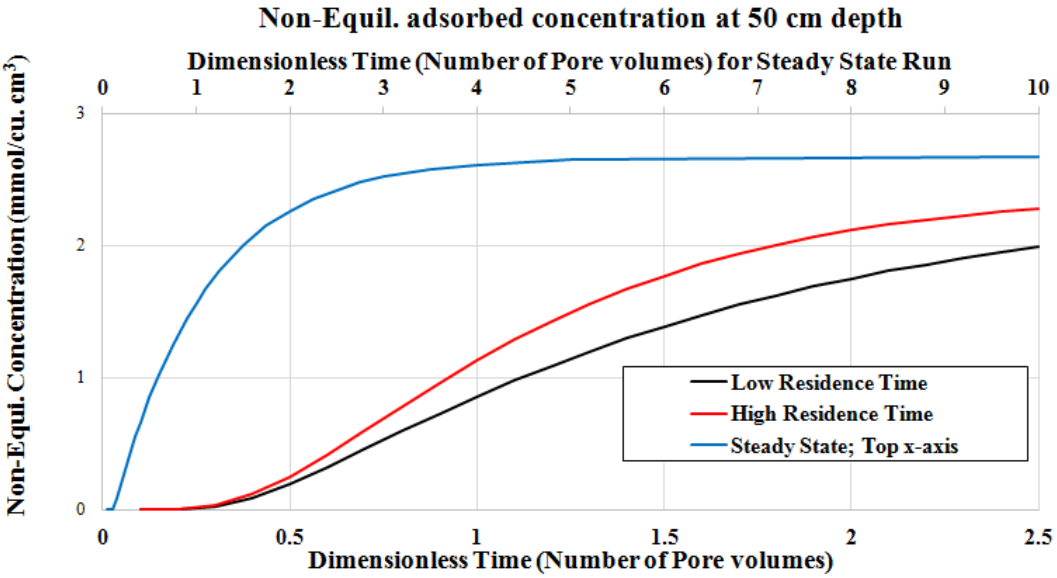

Figure 6c.4. Effect of the resident time on the non-equilibrium sorbed solute concentration.

Example 6d: Advanced Solute Transport: Physical Nonequilibrium (Dual-Porosity) Transport

Example Description and Objectives

Next we use Example 6d to simulate water flow and solute transport through a 100-cm horizontal uniform saturated soil profile having a 20% pressure head gradient imposed across two Constant Pressure Head boundaries. Solute-free water is introduced to the soil profile through the 'Constant Pressure Head' boundary' on the left during the entire 50-day simulation. The soil structure is such that 90% of the pore space is immobile (similarly as often in fractured rock), while the remaining 10% represents the mobile fraction. Physical nonequilibrium is considered with a first-order coefficient (Alpha) controlling the time-dependent solute mass transfer process between the mobile and immobile zones (Figure 6d.1).

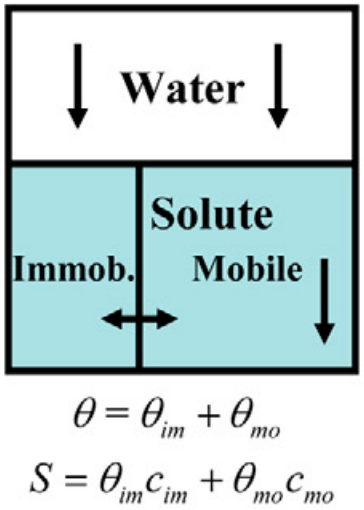

Figure 6d.1. Conceptual physical nonequilibrium model for water flow and solute transport in a dual-porosity medium. In the plots, θ is the water content, θ_{mo} and θ_{im} are water contents of the mobile and immobile flow regions; c_{mo} and c_{im} are concentrations of the corresponding regions, while S is the total solute content of the liquid phase.

Linear sorption is modeled in the mobile phase with a retardation factor $R_m = 1+f\rho K_d/\theta_m = 1+1\times1.5\times0.0267/0.04 = 2.0$ with f (dimensionless) being the fraction of sorption sites in contact with the mobile phase (assumed 1). All other parameters are the same as in Example 6a, except that the mobile phase is only 10% of the total pore space; additionally, we use K_d=0.0267 to maintain R at 2.0. The soil profile has initially a unit solute concentration in the mobile phase. Since R=2.0, an equal mass of solute is initially present in the mobile liquid phase and the sorbed phase. The initial solute concentration in the immobile zone is equal to 0.5 mmol/cm^3. This variable is referred to as 'initial sorbed concentration' in the 'Graphical Editor'. Note that no sorption considered is in the immobile zone since f=1, i.e., all sorption occurs in the mobile liquid zone. This example is not necessarily typical since most of the sorption usually occurs in the immobile phase where smaller pores are in contact with a much larger fraction of the surface area than larger pores. The model formulation used in HYDRUS-1D is based mostly on early work by van Genuchten and Wierenga (1976).

The example illustrates solute transport in a dual-porosity medium subject to physical nonequilibrium whereby time-dependent solute mass transfer takes place between the mobile and immobile zones. The immobile zone represents poorly connected or dead-end pores. The model is well suited to simulate flow and transport in systems with preferential flow paths such as fractured rocks, cracked clays or soils containing macropores due to decayed root channels or earthworm channels (Mallants et al., 1996a, b)

Pre-Processing

Project Manager

- Select *Projects* Tab
- Select *Example 6c1*
- Button “Copy”
- New Name: Example 6d
- Description: Advance Solute Transport - Physical non-equilibrium
- *Button* “OK”
- Select *Example 6d*
- Button “Open”

Main Processes

- Heading: Solute transport with physical non-equilibrium
- Keep unchecked "Water Flow"
- Keep checked "Solute Transport" and "Standard Solute Transport"
- *Button* “OK”

Print Information

- Print Options: Leave as Default
- Number of Print Times: 10
- *Button* “Select Print Times”
- Print Times: 0.5, 1, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50
- *Button* “OK”
- *Button* “Next”

Solute Transport

Non-equilibrium Solute Transport Models

- Check Dual Porosity (Mobile-Immobile Water) Model (Physical non-equilibrium)

Iteration Criteria - Only for Nonlinear Problems

- Absolute Concentration Tolerance: 0 (since this is a linear transport (no non-linear sorption and no blocking), there is no need to specify iteration criteria for solute transport)
- Relative Concentration Tolerance: 0
- Maximum Number of Iteration: 0
- Pulse duration (day)" 0
- *Button* “Next”

Solute Transport Parameters

- Frac. = 1.00 (all sorption sites are in contact with mobile water; perhaps press F1 here for a precise definition of the various parameters)

- Thlmob. = 0.36 (the immobile water content; considering that porosity = 0.4; the mobile water content = (0.4-0.36=) 0.04)
- *Button* "Next"

Solute Transport and Reaction Parameters – Solute 1

- K_d = 0.0267 (cm^3/g)
- Nu = 0 (linear sorption isotherm)
- Beta = 1 (linear sorption isotherm)
- Alpha = 0.02/day (you need to scroll to the right of the table to find this last parameter)
- *Button* "Next"

Solute Transport Boundary Conditions

- Sol. No. 1 Bound. Cond. = 0 $mmol/cm^3$ (no inflow; solute is initially in the soil profile)
- *Button* "Next"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Initial Conditions->Pressure Head
- *Button* (left side) "Edit Condition": select with the Mouse the entire domain and then left click
- Pressure Head Distribution, Top value = 20
  Bottom value = 0; uncheck 'Use top value for both'
- *Button* "OK"
- **Menu**: Conditions->Initial Conditions->Concentration (represents the mobile phase)
- *Button* (left side) "Edit Condition": select with the Mouse the entire profile and then left click the mouse again and specify a concentration 1.0 ($mmol/cm^3$).
- **Menu**: Conditions->Initial Conditions->Sorbed Concentration (for the dual-porosity model, this variable represents the immobile zone)
- *Button* (left side) "Edit Condition": select with the Mouse the entire profile, then left click the mouse again, and specify a concentration of 0.5 ($mmol/cm^3$).
- **Menu**: File->Save Data
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* "Next"

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

Referring to Figure 6d.2:

- A sharp drop occurred in the concentration of the mobile phase during the first 3 days of the simulation. This reflects normal dispersive flow in the mobile

phase with an open (connected) pore structure and a high flow rate, during which most of the solutes in the mobile phase are being leached out.

- After 3 days, a very long tail developed whereby concentrations continued to decrease at a slower rate. This is due to the slow migration of solutes from the immobile zone to the mobile phase owing to the concentration gradient between the immobile and mobile zones (the highest concentration in the immobile zone).

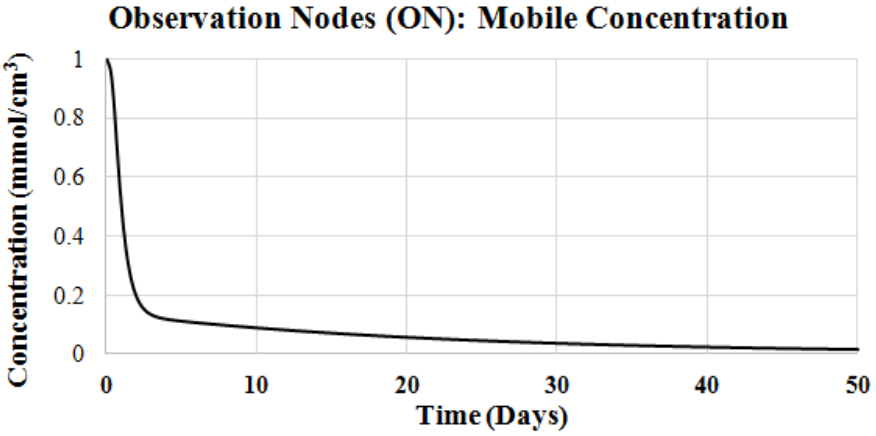

Figure 6d.2 Solute concentration in the mobile phase versus time at a depth of 50 cm.

Profile Information

The concentration profiles in Figures 6d.3 and 6d.4 show sharper fronts in the mobile phase compared to those in the immobile zone since concentrations in the latter decrease more uniformly along the profile as a consequence of the slow rate dictated by the first-order mass transfer parameter.

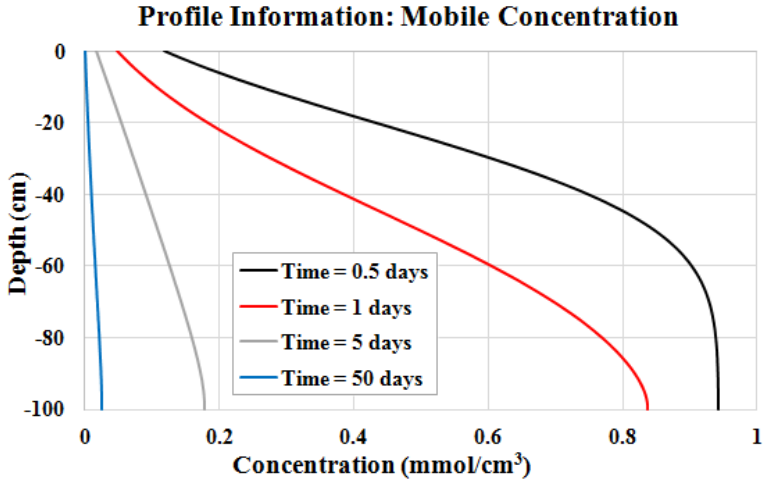

Figure 6d.3 Concentration profiles for the mobile zone at different times.

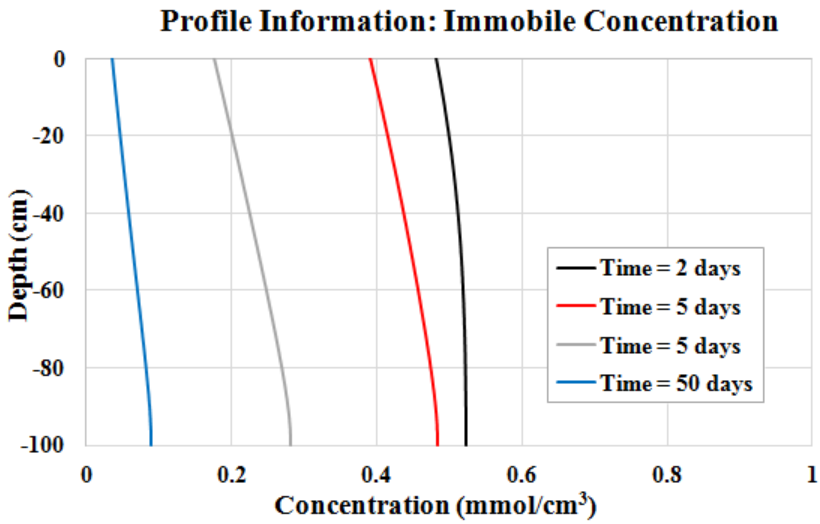

Figure 6d.4. Concentration profiles for the immobile zone at different times.

Solute Fluxes

Referring to Figure 6d.5:

- The nonequilibrium solute flux (i.e., the solute flux between the mobile and immobile regions) slightly increased at the beginning of the simulation reflecting solute migration from the mobile to the immobile zone (since the initial concentration of the mobile zone is higher than that of the immobile zone). Following a rapid drop in the concentration of the mobile phase (due to inflow of solute-free water) as shown in Figure 6d.1, the mass transfer process reverses and solutes move from the immobile to the mobile phase.
- The bottom flux increased at a relatively fast rate at the beginning of the simulation, thus reflecting the steep decrease in the mobile concentration (due to the inlet solute-free flux).
- The two curves become almost parallel at large times since the slow migration of solutes from the immobile zone becomes almost equal to the solute flux across the bottom boundary.

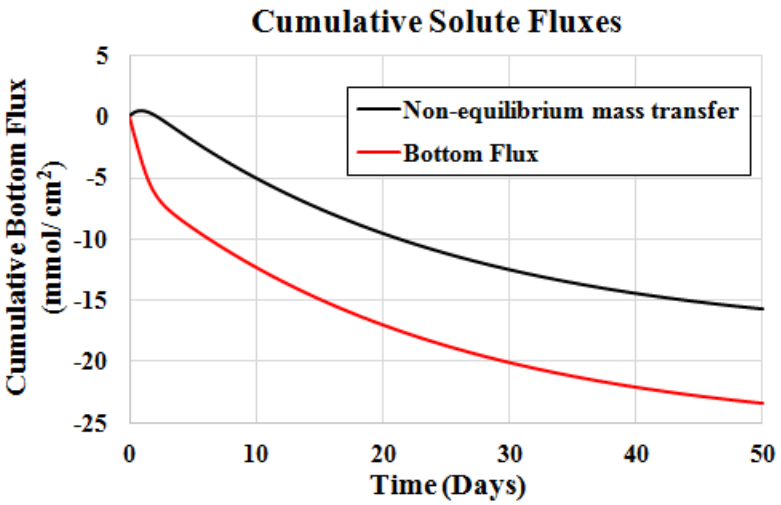

Figure 6d.5. Cumulative solute fluxes.

Mass Balance Information

The mass balance information at Time=0 (initial conditions) is given in Table 6d.1 where:

W-volume	Total water volume in the profile
ConcVol:	Total Solute Mass in equilibrium region (i.e., in the mobile phase and sorption sites in contact with the mobile phase)
ConcVolIm:	Total Solute Mass in nonequilibrium region (i.e., in the immobile liquid zone and sorption sites in contact with this zone)
cMean	Mean concentration in the mobile liquid zone
cMeanIm:	Mean concentration in the immobile liquid zone

Table 6d.1. Mass balance information at Time = 0 (initial conditions).

Time	[days]	0	
Sub-region number			1
Length	[cm]	100	100
W-volume	[cm]	40	40
In-flow	[cm/day]	0	0
hMean	[cm]	10	10
ConcVol	[mmol/cm^2]	8	8
cMean	mmol/cm^2	1	1
ConcVolIm	[mmol/cm^2]	18	18
cMeanIm	mmol/cm^2	0.5	0.5
Top flux	[cm/day]	-4	
Bot flux	[cm/day]	-4	

Interpretation of initial (at Time=0) solute masses (ConcVol and ConcVolIm) in the Mass Balance File

W-volume = Qs × L = 0.40 × 100 =40 cm

ConcVol, S_m

Initial concentration in the mobile zone, C_m = 1 mmol/cm^3
Thlmob. (the immobile water content, θ_{im}) = 0.36 cm^3/cm^3
The mobile water content, θ_m = Qs – ThImob = 0.40 – 0.36 = 0.04 cm^3/cm^3
Length of the soil profile, L = 100 cm
Bulk Density, ρ = 1.5 g/cm^3
The distribution coefficient, K_d = 0.0267 cm^3/g
Fraction of sorption sites in contact with the mobile zone, f = 1
$S_m = C_m(f\rho K_d+\theta_m)L$=1×(1×1.5×0.0267+0.04)×100=8.005 mmol/cm^2

ConcVolIm, S_{im}

Initial concentration in immobile zone C_{im} = 0.50 mmol/cm^3
$S_{im}=C_{im}[(1-f)\rho K_d+\theta_{im})L$=0.5×(0×1.5×0.0267+0.36) ×100=18 mmol/cm^2

Example 6e: Advanced Solute Transport: Combined Physical and Chemical Nonequilibrium

Example Description and Objectives

Example 6e simulates water flow and solute transport through a 100-cm horizontal uniform saturated soil profile having a 20% pressure head gradient imposed across two Constant Pressure Head boundaries. Water with a solute concentration of 2 mmol/cm^3 is introduced into the soil profile through the upper (left) 'Constant Pressure Head' boundary' during the entire 50-day simulation. The soil structure is such that 50% of the pore space (θ_s =0.4) is immobile (θ_{im} =0.2). **Physical nonequilibrium** is modeled using a first-order mass transfer coefficient (Alpha) that controls time-dependent solute mass transfer between the mobile and immobile zones. All sorption sites are assumed to be in contact with the mobile phase (f=1) and are split into those subjected to equilibrium sorption (10%; FracM=0.1) and those with kinetic sorption (90%). Equilibrium sorption is modeled using equilibrium (instantaneous) linear sorption with R=2.0. Kinetic sorption (**chemical nonequilibrium**) is modeled using a first-order coefficient (Omega) that controls time-dependent solute mass transfer between the liquid phase and the sorption sites of the mobile zone (see Figure 6e.1). The soil profile initially has a unit solute concentration in the mobile zone, which implicitly implies that an equal mass of sorbed solutes is initially present on the equilibrium sorption sites (to honor the linear sorption isotherm with R=2.0). Initial solute concentration in the immobile zone is equal to 0.5 mmol/cm^3. Note that after a sufficiently long run time, the profile reaches a steady-state situation whereby non-equilibrium sites do reach equilibrium and thus satisfy the condition imposed by the linear sorption isotherm with R=2.0 (solute masses in the liquid mobile and sorbed mobile phases become equal).

This example demonstrates solute transport with combined physical and chemical non-equilibrium whereby time-dependent solute mass transfer takes place between the mobile and immobile zones, in combination with instantaneous and time-dependent mass transfer between the liquid phase and sorption sites of the mobile zone.

Pre-Processing

Project Manager

- Select *Projects* Tab
- Select *Example 6d*
- Button "Copy"
- New Name: Example 6e
- Description: Solute transport with physical and chemical non-equilibrium
- *Button* "OK"
- Select *Example 6e*
- Button "Open"

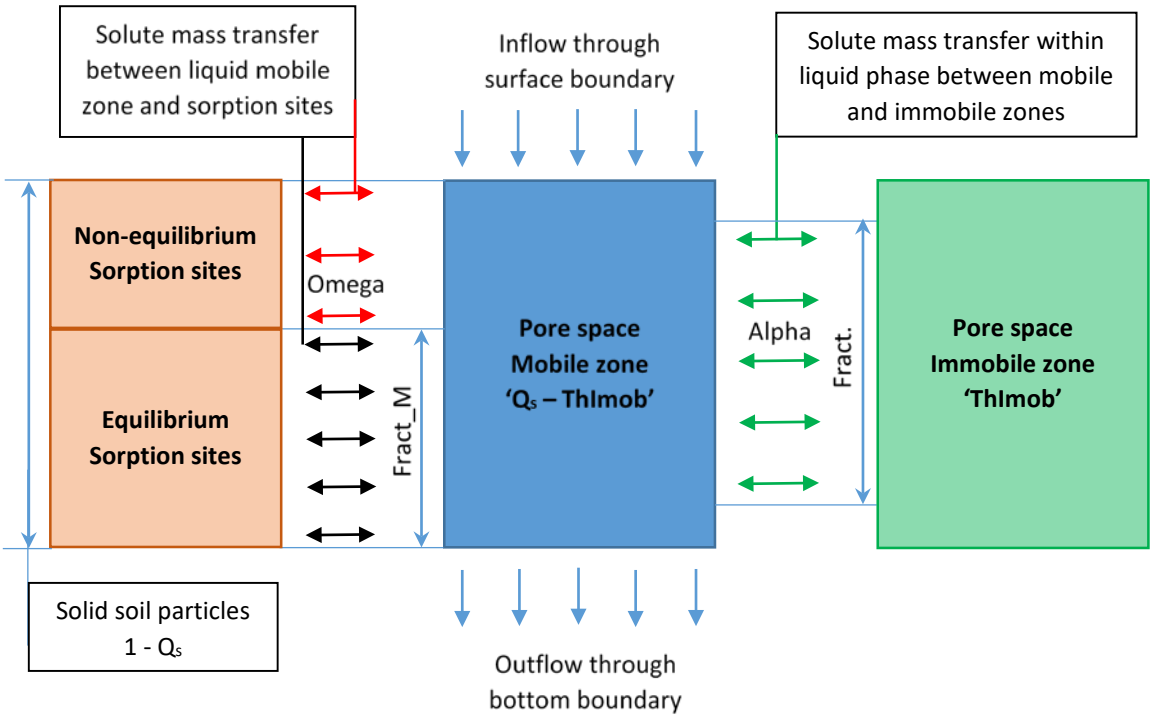

Figure 6e.1. Conceptualization of the dual-porosity model with two-site sorption in the mobile zone.

Main Processes

- Heading: Solute transport with physical and chemical non-equilibrium
- *Button* "Next"

Geometry Information

- Number of Layers for Mass Balance: 2 (to obtain the mass balance of each soil layer)
- *Button* "Next"

Print Information

- Print Options: Leave as Default
- Number of Print Times: 25
- *Button* "Select Print Times"
- *Button* "Default"
- *Button* "OK"
- *Button* "Next"

Solute Transport

Non-equilibrium Solute Transport Models

- Check Dual Porosity Model with Two-Site Sorption in the Mobile Zone (Physical and Chemical non-equilibrium)
- Pulse duration (day) 50
- *Button* "Next"

Solute Transport Parameters

- Disp = 10 cm
- Frac. = 1.00 (all sorption sites are in contact with mobile water)
- Thlmob. = 0.20 (immobile water content)
- *Button* "Next"

Solute Transport and Reaction Parameters – Solute 1

- K_d = 0.133 (cm^3/g)
- Nu = 0 (linear sorption)
- Beta = 1 (linear sorption)
- Frac_M = 0.10 (scroll to the right to find this parameter; fraction of sorption sites in contact with the mobile region that are subject to instantaneous sorption)
- Omega = 0.50 day^{-1} (first-order mass transfer coefficient representing kinetic sorption)
- α = 0.02 day^{-1} (first-order mass transfer coefficient representing mass transfer between mobile and immobile zones)
- *Button* "Next"

Solute Transport Boundary Conditions

- Sol. No. 1 Bound. Cond. = 2 $mmol/cm^3$
- *Button* "Next"

Soil Profile – Graphical Editor

- **Menu**: Conditions->Subregions
- *Button* (left side) "Edit Condition", select with the Mouse node 51, left click the mouse
  Material Index: 2 (this will select a 1-cm element located at a depth of 50-51 cm)
- **Menu**: File->Save Data
- **Menu**: File->Exit

Execute HYDRUS-1D

- **Menu**: Calculation->Execute HYDRUS-1D or a **Toolbar** button  .

Post-Processing

Observation Points

Referring to Figure 6e.2:

- An initial drop occurs in concentrations at both observation points as solutes migrate from the mobile to the immobile region, thus reducing the concentration in the former.
- After about 1 and 3 days, solutes introduced at the upper Constant Pressure Head boundary reach the depths of 50 cm and 100 cm, respectively, thus increasing concentrations.
- At 50 days, concentrations at both observation points almost reach a steady-state (approaching 2 $mmol/cm^3$, which is equal to the inlet concentration at the upper boundary).

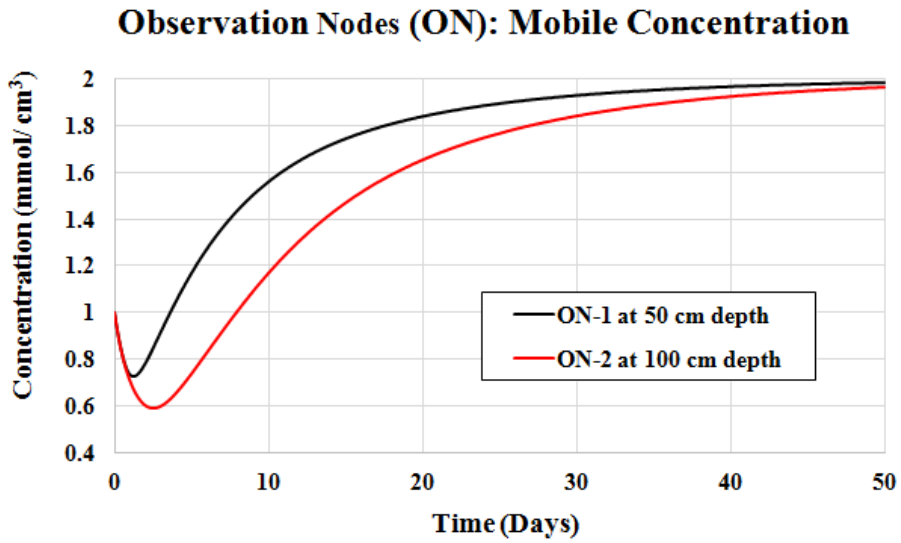

Figure 6e.2. Solute concentrations in the mobile region versus time at depths of 50 and 100 cm.

Profile Information:

Referring to Figure 6e.3, which shows concentration profiles in the mobile zone at 0, 2, and 50 days:

- The initial profile (Time = 0) has a uniform initial unit concentration of 1 mmol/cm^3 in the mobile zone.
- After 2 days, the concentration near the upper (surface) boundary increases due to the solute (2 mmol/cm^3) inflow at the constant pressure head boundary. At this early time, the concentration increase was restricted to the top 40 cm of the profile. Concentrations below this point continue decreasing due to the migration of solutes from the mobile to the immobile zone (as noted in Figure 6e.1) at early times.
- At 50 days, the concentration profile near the surface (the top 23 cm) has already reached the steady-state concentration of 2 mmol/cm^3. The concentration in the rest of the soil profile is slightly lower (1.96 mmol/cm^3 at the 100-cm depth).

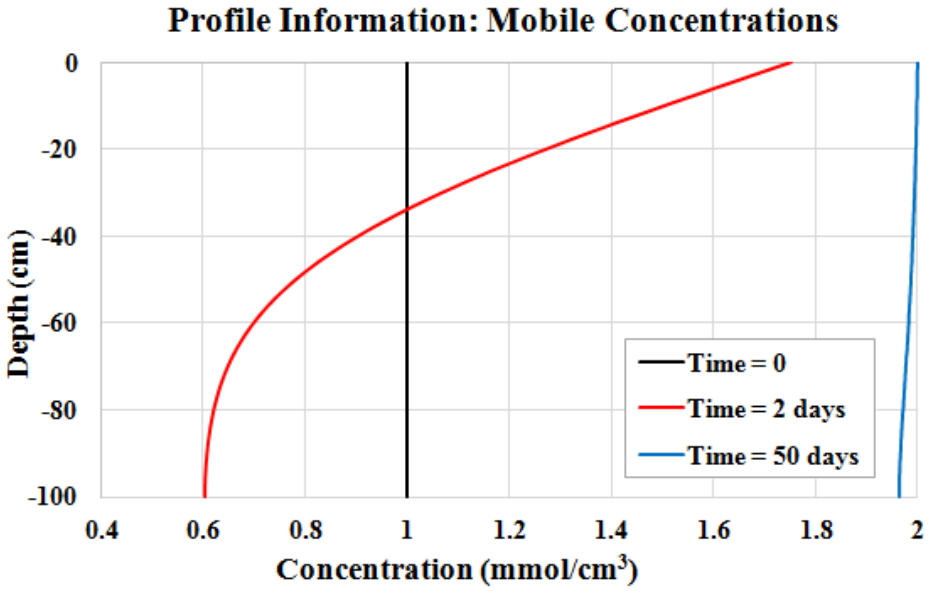

Figure 6e.3. Concentration profiles in the mobile zone at different times.

Referring to Figure 6e.4, which shows concentration profiles in the immobile zone at 0, 2, and 50 days:

- The initial profile (Time = 0) has a uniform concentration of 0.5 mmol/cm^3 in the immobile zone.
- After 2 days, concentrations in the immobile zone slowly increase across the entire profile. In the lower 40 cm, there is a linear increase driven by the first-order mass transfer parameter (Omega). Note that the straight line is parallel with the initial condition (Time=0). The top 50 cm, however, displays a nonlinear concentration profile resulting from a higher migration of solutes from the mobile zone as driven by the concentration gradient caused by the inlet concentration of 2 mmol/cm^3 at the constant pressure head boundary. Had this gradient been absent, concentrations would have been constant throughout the entire profile (represented by a dotted red line).
- At 50 days, the concentration profile has not yet reached the steady-state concentration of 2 mmol/cm^3 due to slow migration of solutes from the mobile zone.

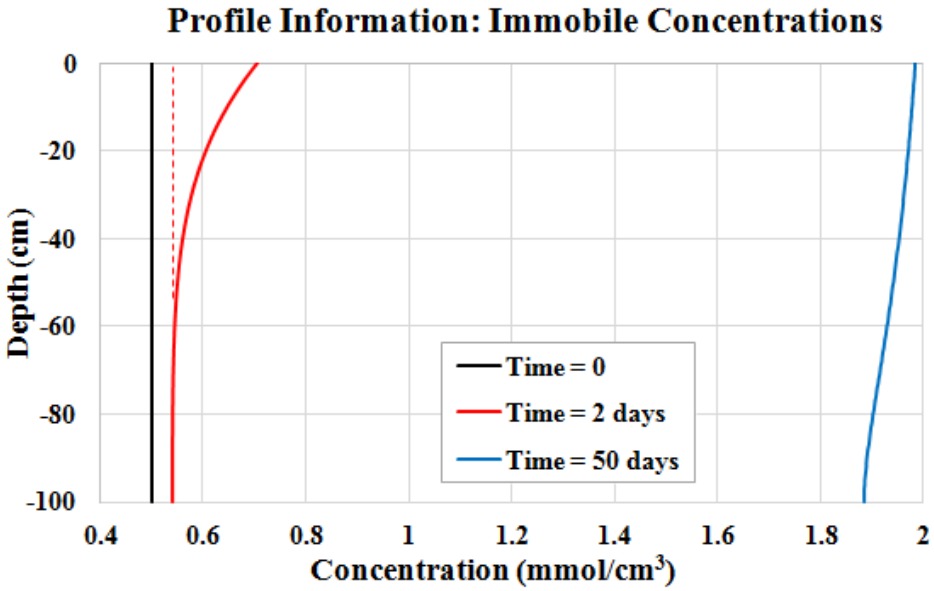

Figure 6e.4. Concentration profiles in the immobile zone at different times.

Solute Fluxes

Referring to Figure 6e.5:

- The cumulative non-equilibrium mass transfer represents the sum of mass transfer between the mobile and immobile zones, and mass transfer between the liquid phase and chemical non-equilibrium sorption sites (i.e., mass transfer from the equilibrium phase to the nonequilibrium phase). It seems that non-equilibrium mass transfer has almost approached a steady-state (since the blue line is almost horizontal) (as also indicated by Figs 6e.3 and 6e.4.
- The cumulative surface and bottom fluxes will be used to check against solute masses reported in the Mass Balance Information.

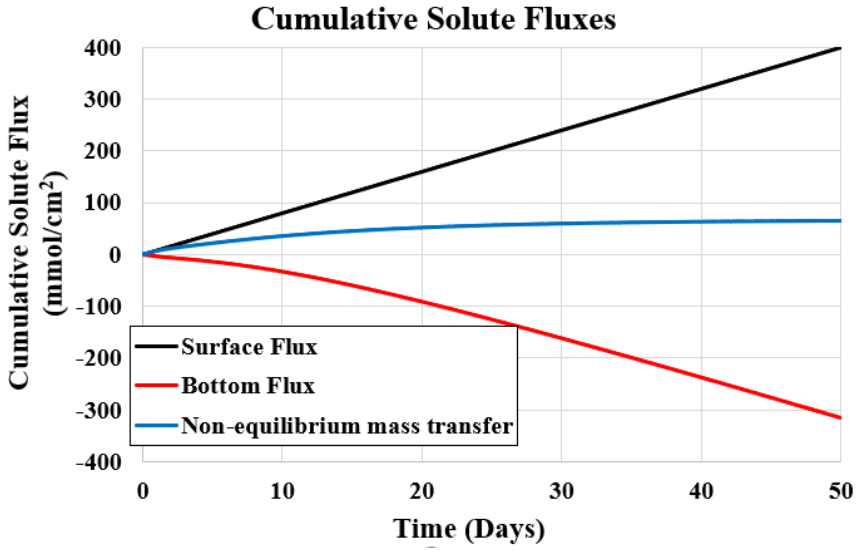

Figure 6e.5. Cumulative solute fluxes versus time.

Mass Balance Information

- Mass balance information at Time=0 (initial conditions) and Time=50 days for the entire soil profile is given in Table 6e.1 where:

W-volume Total water volume in the profile
ConcVol Total solute mass in equilibrium phases, i.e., the mobile liquid phase and equilibrium sorption sites of the mobile zone (this excludes the mass in the immobile liquid phase and non-equilibrium sites of the mobile zone).
cMean Mean concentration of the mobile liquid phase
ConcVolIm Total solute mass of the immobile liquid phase
cMeanIm Mean concentration of the immobile liquid phase
SorbVolIm2 Total solute mass of non-equilibrium sorption sites of the mobile zone

Table 6e.1. Mass balance information for the entire profile at various times.

Time (Days)		0	50	Steady State
Sub-region number			1	
Length	[cm]	100		
W-volume	[cm]	40		
In-flow	[cm/day]	0	0	0
hMean	[cm]	10	10	10
ConcVol	[mmol/cm^2]	**21.995**	**43.63**	**44**
cMean	[mmol/cm^3]	1.0	1.98	2
ConcVolIm	[mmol/cm^2]	**10**	**38.75**	**40**
cMeanIm	[mmol/cm^3]	0.5	1.93	2
SorbVolIm2	[mmol/cm^2]	**0**	**35.56**	**36**

- Interpretation of solute masses (ConcVol, ConcVolIm and SorbVolIm2) in the Mass Balance Information

Referring to Table 6e.1:

<u>At Time=0</u>

ConcVol

Initial concentration in the mobile zone, C_m = 1 mmol/cm^3
Thlmob. (immobile water content, θ_{im}) = 0.20 cm^3/cm^3
Mobile water content, θ_m = Qs – ThImob = 0.40 – 0.20 = 0.20 cm^3/cm^3
Length of the soil profile, L = 100 cm
Bulk Density, ρ =1.5 g/cm^3
Distribution coefficient, K_d = 0.133 cm^3/g
Retardation factor of the mobile zone:
$R_m=1+f\rho K_d/\theta_m=1+1\times1.5\times0.133/0.20=2.0$

The fraction of sorption sites in contact with the mobile zone, f=1
The fraction of sorption sites in contact with the mobile zone that is at equilibrium, f_m=0.1
$S_m=C_m(ff_m\rho K_d+\theta_m)L$=1×(1×0.1×1.5×0.133+0.20) ×100=22 mmol/cm^2

ConcVolIm

Initial concentration of the immobile zone C_{im} = 0.50 mmol/cm^3
$S_{im}=C_{im}[(1-f)\rho K_d+\theta_{im})L$=0.5×(0×1.5×0.133+0.20) ×100=10 mmol/cm^2

SorbVolIm2

Initial sorbed mass of chemical non-equilibrium sites is equal to zero

At Time=50 days (compare with flux data)

From Mass Balance data:
Net mass of solutes added to a profile after 50 days = Solute mass at 50 days – initial solute mass
= (43.63+38.75+35.56) – (22+10) = **85.94** mmol/cm^2
Non-equilibrium mass transfer between mobile and immobile zones = 38.75-10 = 28.75 mmol/cm^2
Non-equilibrium sorption mass transfer = 35.56-0.0 = 35.56 mmol/cm^2
Total non-equilibrium mass transfer = 28.75 + 35.56 = **64.31** mmol/cm^2

From Solute Flux data:
Cumulative Surface Solute Flux = 400 mmol/cm^2
Cumulative Bottom Solute Flux = -314.43 mmol/cm^2
Net mass of solutes added to profile after 50 days = 400 – 314.43 = **85.57** mmol/cm^2
Cumulative non-equilibrium mass transfer = **64.31** mmol/cm^2

Note that the small discrepancy in the total solute mass added is reflected in the error term (CncBalT) in the Mass Balance information.

At steady state:

ConcVol = 44 mmol/cm^2, comprising 40 mmol/cm^2 in the liquid mobile phase and 4 mmol/cm^2 in the sorbed mobile phase.

SorbVolIm2 is equal to 36 mmol/cm^2

Total sorbed mass (equilibrium + non-equilibrium sites) = 4 + 36 = 40 mmol/cm^2

Total sorbed mass = total mass in the liquid phase, which satisfies R=2 as an equilibrium state has been reached.

- Figure 6d.6 shows the solute breakthrough in the immobile zone at a depth of 50 cm using data collated from the Mass Balance Information File (cMeanIm for Subregion 2).

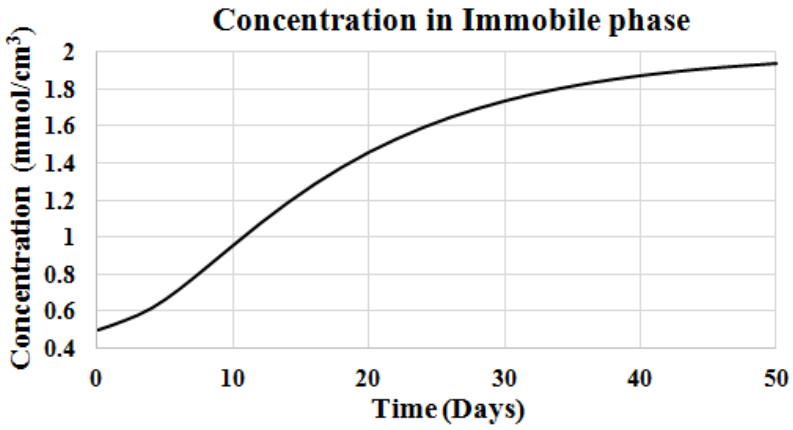

Figure 6e.6. Immobile solute concentrations versus time at a depth of 50 cm.

- Figure 6d.7 shows the individual mass transfer for the physical (ConcVolIm) and chemical (SorbVolIm2) non-equilibrium regions. If the initial solute mass in the immobile zone (10 mmol/cm^2) is deducted from the physical non-equilibrium mass values (red line), and then added to the chemical non-equilibrium mass (black line), it will yield the total non-equilibrium mass transfer reported in Figure 6e.4 (blue line).

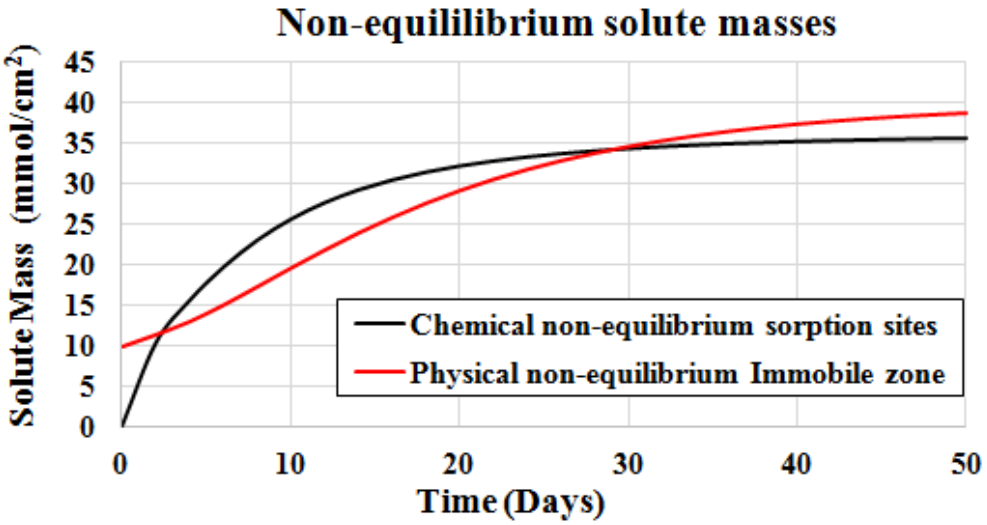

Figure 6e.7. Non-equilibrium solute masses versus time.

Example 7a: Inverse Modeling: One-Step Outflow Method

Example Description and Objectives

Example 7a considers the inverse solution for a one-step outflow experiment (Figure 7a.1). Data presented by Kool et al. (1985) and used in Example 6 of the HYDRUS-1D manual (p. 170) are used in the analysis.

An undisturbed core sample, having a length of 3.95 cm and a diameter of 5.4 cm, was equilibrated at near-saturated conditions in a Tempe pressure cell. The retention curve was first measured for pressure heads up to -10 m. Water contents at pressure heads of -30 and -150 m were measured on disturbed samples. After resaturation, a pneumatic pressure of 10 m was imposed at the top of the sample, and the cumulative outflow was recorded with time. The position of the measuring burette was adjusted manually every time reading was made to maintain a constant head lower boundary condition. At the end of the experiment, the soil was resaturated, and the saturated hydraulic conductivity of the soil and porous plate were measured with a falling head method.

Three hydraulic parameters (α, n, and θ_r) are to be estimated by numerical inversion of the observed cumulative outflow data and the measured water content at a pressure head of -150 m. Since water exits the soil column across a ceramic plate, the flow problem involves a two-layered system. To be able to simulate flow through the ceramic bottom plate without having to modify the code, the HYDRUS model must be able to simulate flow through materials with very high air entry values such that the ceramic plate remains saturated at all times during the outflow experiment. A very high air entry value of the plate was ensured by specifying parameter α to be 10^{-20} (1/cm). The soil profile, which consists of a 3.95-cm long soil sample and a 0.57-cm thick ceramic plate, was discretized into 50 nodes with five nodes representing the ceramic plate. Only a few nodes were used for the ceramic plate since the plate remained saturated during the entire experiment, thus causing the flow process in the plate to be linear.

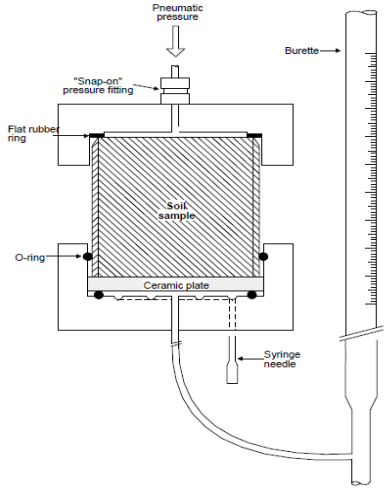

Figure 7a.1. Schematic of the one-step outflow measurement device (from Green et al., 1998).

Pre-Processing

Project Manager

- Click *Button* "New"
- Type Name: Onestep
- Type Description: Onestep Outflow Method
- *Button* "OK"

Main Processes

- Heading: Onestep Outflow Method
- Check "Inverse Solution"
- *Button* "Next"

Inverse Solution

When the option "Inverse Solution" is selected in the Main Processes window, the next dialog that appears is the "Inverse Solution" dialog window (Fig. 7a.2). In this window, you must first select which parameters are to be estimated (*Estimate* …). One can estimate either a) soil hydraulic parameters, b) solute transport parameters, c) heat transport parameters, or any combination of these three sets of parameters. When only water flow is simulated, then only soil hydraulic parameters can be optimized, and the other sets of parameters (i.e., for solute and heat transport) are disabled.

You must also select the method of **Weighting of Inversion Data** in the objective function. One can choose between no weighting, weighting by mean ratios (of different data types in the objective function), or weighting by standard deviations. When no weighting is selected, users need to supply weights for particular data points in the **Data for Inverse Solution** dialog window (Fig. 7a.4). When weighting by mean ratio or standard deviation is selected, the code will calculate either means or standard deviations for different data sets (e.g., water contents, pressure heads, concentrations, …), and then adjust the weights proportionally. These internal weights can still be multiplied by weights from the **Data for Inverse Solution** dialog window.

The objective function for the inverse estimation of solute transport parameters can be defined using different types of concentrations. Available **Concentration Types** are: a) the resident concentration in the liquid phase, b) a log-transformation of the resident concentration in the liquid phase, c) the outflow (flux) concentration, d) the solute concentration flux, e) the cumulative concentration (solute) flux, and f) the total resident concentration. The total resident concentration includes concentrations in the sorbed and nonequilibrium phases.

The maximum number of iterations for the inverse solution is also specified in this dialog window. If you select a zero for the number of iterations, then only the direct simulation is carried out. However, you can then still enter the measured data, in which case the code compares results of the direct simulation with the measured data.

HYDRUS allows users to optimize up to 15 parameters (NPaD is the maximum allowed number of optimized parameters). We, however, do not recommend optimizing so many parameters simultaneously. Unsaturated flow problems are inherently ill-posed, and thus not too many parameters can be successfully optimized simultaneously. When more parameters are optimized, the problem often becomes nonunique. The problems

of unsaturated flow are different than those of saturated flow where it is common to optimize many more parameters simultaneously. For details see Šimůnek and Hopmans (2002), Hopmans et al. (2002), and Šimůnek et al. (2002).

Finally, the "Number of Data Points in Objective Function" must be specified. This is the total number of all data points that will be considered in the objective function. This number needs to be specified in the **Data for Inverse Solution** dialog window (Fig. 7a.4).

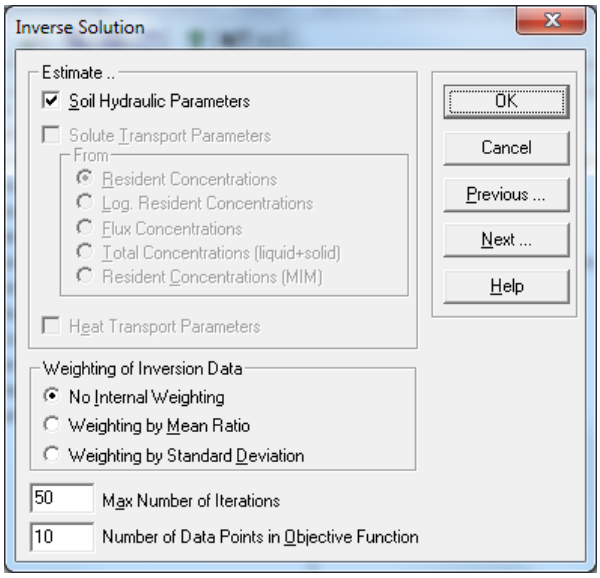

Figure 7a.2. The **Inverse Solution** dialog window.

- Check "Soil Hydraulic Parameters"
- Check "No Internal Weighting" (we want to replicate the example in the same way as originally solved by Kool et al. (1985)
- Max. Number of Iterations: 20
- Number of Data Points: 10
- *Button* "Next"

Geometry Information

- Number of Soil Materials: 2 (soil itself and the ceramic plate)
- Number of Layers for Mass Balances: 2 (ditto)
- Depth of the Soil Profile (cm): 4.52
- *Button* "Next"

Time Information

- Time Units: Hours
- Final time (hour): 100
- Initial Time Step (hour): 0.001
- Minimum Time Step (hour): 0.0001
- Maximum Time Step (hour): 10
- *Button* "Next"

Print Information

- Uncheck "Screen Output"
  (since the direct simulations are carried out many times during the inverse parameter estimation process, we are not interested in detailed information about each run, but only in information printed after each inverse solution iteration, such as the value of the objective function and values of optimized parameters)
- Number of Print Times: 11
- *Button* "Select Print Times": 0.017, 0.033, 0.05, 0.167, 0.5, 1.33, 2.75, 5.417, 10, 15, 100
- *Button* "Next"

Water Flow - Iteration Criteria

- Water Content Tolerance: 0.0001
- Pressure Head Tolerance (cm): 0.1
- Upper Limit of the Tension Interval: 15000 (to extend the Internal Interpolation Tables all the way to the lowest recorded value, i.e., the wilting point).
- *Button* "Next"

Water Flow - Soil Hydraulic Model

- Leave as Default
- *Button* "Next"

Water Flow - Soil Hydraulic Parameters

When the soil hydraulic parameters are optimized, a different version of the Water Flow Parameters dialog window (Fig. 7a.3) appears. In this window, which appears for each soil material, you must provide initial estimates of the optimized soil hydraulic parameters, specify which parameters are to be optimized (check the appropriate boxes), and provide parameter constraints for the optimization. Entering zeros (the default values) for the minimum and maximum constraints signifies that the parameters are unconstrained. Initial values specified for parameters that are not optimized will be kept constant during the inverse optimization process.

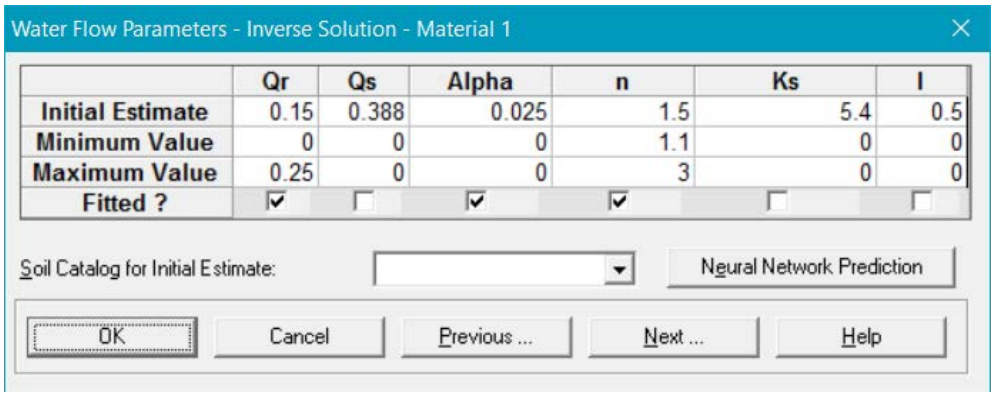

Figure 7a.3. The **Water Flow Parameters - Inverse Solution** dialog window.

- Initial Estimate: θ_r=0.15, θ_s=0.388, α=0.025, n=1.5, K_s=5.4, l= 0.5
- Fitted: θ_r, α, and n
- Second Material: θ_r=0., θ_s=1., α=1e-20, n=1.001, K_s=0.003, l= 0.5
- *Button* "Next"

Water Flow - Boundary Conditions

- Upper Boundary Condition: Constant Flux
- Lower Boundary Condition: Constant Pressure Head
- *Button* "Next"

Water Flow - Constant BC

- Upper Boundary Flux: 0
- *Button* "Next"

Data for Inverse Solution

In the table **Data for Inverse Solution** (Fig. 7a.4) you must specify the measured data that define the objective function to be minimized during the parameter optimization process. Many different types of data can be used to define the objective function. How the values in the **X** and **Y** columns are interpreted depends on the **Type** and **Position** values. **Weight** is the weight associated with a particular data point. Table 7a.1 lists selected data types that can be included in the objective function. A complete list of various data types that can be used to define the objective function and how the X and Y columns are interpreted is given in the online help and in the manual of HYDRUS-1D. You can double-check the correct definition of the data types by clicking on 'Show list boxes (not recommended for large data sets' at the bottom of the window.

Table 7a.1. Data types for the objective function (Inverse Problem).

Type	Data Point
0	Cumulative boundary fluxes across a specified boundary
1	Pressure head measurements at selected observation point(s)
2	Water content measurements at selected observation point(s)
3	Boundary flow across a specified boundary
4	Concentration or temperature measurements at observation point(s)
5	$h(\theta)$ measurements, data point of the retention curve
6	$K(h)$ measurements, data point of the hydraulic conductivity function
7	Prior knowledge of parameter α
8	Prior knowledge of parameter n
9	Prior knowledge of parameter θ_r
10	Prior knowledge of parameter θ_s
11	Prior knowledge of parameter K_s

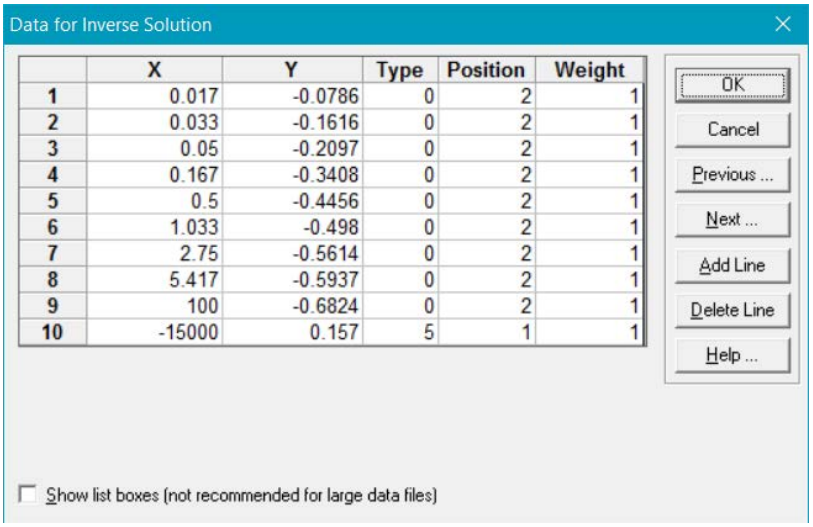

Figure 7a.4. The **Data for Inverse Solution** dialog window.

The first nine data points in this example are interpreted in the program as (Type=0) cumulative outflow *Q* (column Y) at time *t* (column X) through the bottom boundary (Position=2). Cumulative outflow values are negative because outflow is downward (against the *z* axis). The last (10th) value is interpreted as (Type=5), i.e., a data point of the retention curve (water content θ (column Y) at pressure head *h* (column X) for material 1 (Position=1)).

- Enter the following data (copy from the Excel file)

0.017	-0.0786	0	2	1
0.033	-0.1616	0	2	1
0.05	-0.2097	0	2	1
0.167	-0.3408	0	2	1
0.5	-0.4456	0	2	1
1.033	-0.498	0	2	1
2.75	-0.5614	0	2	1
5.417	-0.5937	0	2	1
100	-0.6824	0	2	1
-15000	0.157	5	1	1

- *Button* "Next"

Soil Profile - Graphical Editor

- **Menu:** Options->Grid or **Toolbar** : Height: 0.05
- **Menu:** Condition->Profile Discretization or **Toolbar**
- *Button* (Edit Bar) "Number": 50
- *Button* (Edit Bar) "Insert Fixed" at 3.95 cm
- *Button* (Edit Bar) "Density": deselect "Use upper", upper density =0.1 at 3.95 cm
- **Menu:** Condition->Initial Condition->Pressure Head or **Toolbar**
- *Button* (Edit Bar) "Edit Condition"
- Select entire profile: Top value=-2, Bottom value=2.52
  Deselect "Use top value for both"
- Select the lowest node = -1000 cm

- **Menu:** Condition->Material Distribution or **Toolbar** 
- *Button* (Edit Bar) "Edit Condition"
- Select the ceramic plate and specify "Material Index"=2
- Ditto for "subregions"
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile - Summary

- *Button* "Next"

Execute HYDRUS

- **Menu**: Calculation->Execute HYDRUS or a **Toolbar** button  .

Post-Processing

Figure 7a.5 shows the measured cumulative outflow curve versus time, as well as the best fit obtained with HYDRUS-1D. Initial and final parameter estimates are listed in Table 7a.2. Notice the very good fit of the measured data in Figure 7a.5, with R^2 being 0.9987. Figure 7a.6 shows a comparison of the predicted and measured retention curves, as well as a comparison of the diffusivity curve obtained by parameter estimation and $D(\theta)$ values calculated independently using the method of *Passioura* [1976]. Again, notice the close agreement between predicted and measured values.

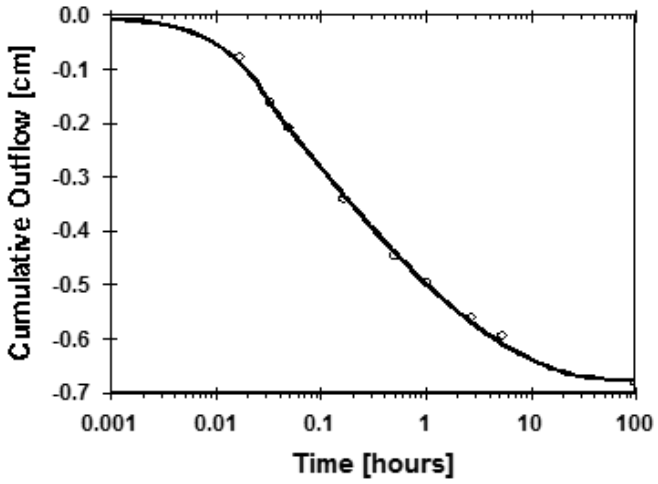

Figure 7a.5. Measured and optimized cumulative outflow versus time for the one-step outflow experiment.

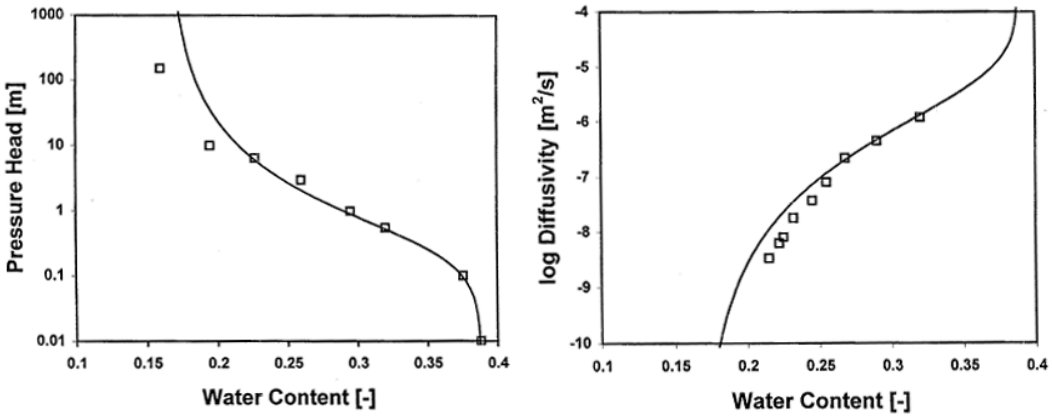

Figure 7a.6. Observed and predicted retention curves (left) and calculated and predicted diffusivities (right).

Table 7a.2. Initial estimates of and optimized parameters for one-step outflow experiment.

Parameter	Initial Estimate	Final Value
θ_r [cm^3/cm^3]	0.15	0.166
θ_s [cm^3/cm^3]	0.388$^+$	
α [1/cm]	0.025	0.0363
n [-]	1.5	1.42
K_s [cm/h]	5.4$^+$	
$K_{s,cer}$ [cm/h]	0.003$^+$	
l [-]	0.5$^+$	

$^+$ Not optimized

Example 7b: Inverse Modeling: Multi-Step Outflow Method

Example Description and Objectives

Although initial applications of the inverse approach to one-step outflow data appeared promising, later studies revealed possible problems in terms of non-uniqueness of the optimized parameters (e.g., van Dam et al., 1992, 1994). To circumvent uniqueness problems, van Dam et al. (1994) conducted and analyzed outflow experiments in which the pneumatic pressure was increased in several smaller steps. Eching and Hopmans (1993) similarly estimated soil hydraulic parameters from simultaneous measurements of transient cumulative outflow and the soil water pressure head inside of the soil sample during a multistep outflow experiment.

In this test example, we analyze a multistep outflow experiment with simultaneous measurement of the pressure head inside the soil sample (Hopmans, personal communication). The experimental setup consisted of a 6-cm long soil column in a Tempe pressure cell modified to accommodate a micro-tensiometer-transducer system. A tensiometer was installed, with the cup centered 3 cm below the soil surface. The soil sample was saturated from the bottom and subsequently equilibrated to an initial soil water pressure head of -25 cm at the soil surface. Pressures heads of -100, -200, -400, and -700 cm were applied subsequently in consecutive steps at 0, 12.41, 48.12, and 105.92 hours, respectively.

Pre-Processing

Project Manager

- *Button* "New"
- Name: Multistep
- Description: Multistep Outflow Method
- *Button* "OK"

Main Processes

- **Heading**: Multistep Outflow Method
- Check "Inverse Solution"
- *Button* “Next”

Inverse Solution

- Check "Soil Hydraulic Parameters"
- Check "Weighting by Standard Deviations"
- Max. Number of Iteration: 50
- Number of Data Points: 229
- *Button* “Next”

Geometry Information

- Length Units: cm
- Number of Soil Materials: 1
- Number of Layers for Mass Balances: 1
- Depth of the Soil Profile: 6.0

- *Button* “Next”

Time Information

- Time Units: Hours
- Final time (hours): 190.384
- Initial Time Step (hours): 0.01
- Minimum Time Step (hours): 0.0001
- Maximum Time Step (hours): 120
- Check Time-Variable Boundary Conditions
- Number of Time-Variable Boundary Records: 4
- *Button* “Next”

Print Information

- Uncheck "Screen Output"
- Number of Print Times: 10
- *Button* "Select Print Times": 0.01, 0.1, 0.2, 19.038, 38.077, 57. 115, 133, 27, 152.31, 171.35, 190.384
- *Button* “Next”

Water Flow - Iteration Criteria

- Leave the default values
- *Button* “Next”

Water Flow - Soil Hydraulic Model

- Leave the default model
- *Button* “Next”

Water Flow - Soil Hydraulic Parameters

- Initial Estimate: Select Loam from the Catalog for Initial Estimate
- Fitted: All six parameters
- *Button* “Next”

Water Flow - Boundary Conditions

- Upper Boundary Condition: Constant Flux
- Lower Boundary Condition: Variable Pressure Head
- *Button* “Next”

Water Flow - Constant BC

- Upper Boundary Flux: 0
- *Button* “Next”

Variable Boundary Conditions

- Enter the following values:

Time	**GWL**
12.42	-100
48.12	-200
105.92	-400
190.384	-705

- *Button* “Next”

Data for Inverse Solution

- Copy from the Excel File: Worksheet HYDRUS-1D (One-Step)
- *Button* "Next"

Soil Profile - Graphical Editor

- **Menu:** Condition->Profile Discretization or **Toolbar**
- *Button* (Edit Bar) "Number": 50
- *Button* (Edit Bar) "Insert Fixed" - at -3 cm
- *Button* (Edit Bar) "Density": Select the top node and specify Density=3
- *Button* (Edit Bar) "Density": Select the middle node (-3 cm) and set Density=2
- **Menu:** Condition->Initial Condition->Pressure Head or **Toolbar**
- *Button* (Edit Bar) "Edit condition"
- Select entire profile: Top value=-25, Bottom value=-19
- Deselect "Use top value for both"
- **Menu**: Conditions->Observation Points or **Toolbar**
- *Button* (Edit Bar) "Insert": Set Observation Point at -3 cm
- **Menu**: File->Save Data or **Toolbar**
- **Menu**: File->Exit

Soil Profile - Summary

- *Button* "Next"

Execute HYDRUS

- **Menu**: Calculation->Execute HYDRUS or a **Toolbar** button .

The computations (using the inverse computational module h1d_clci.exe) are now being carried out, with parts of the results being displayed in a DOS window (Fig. 7b.1).

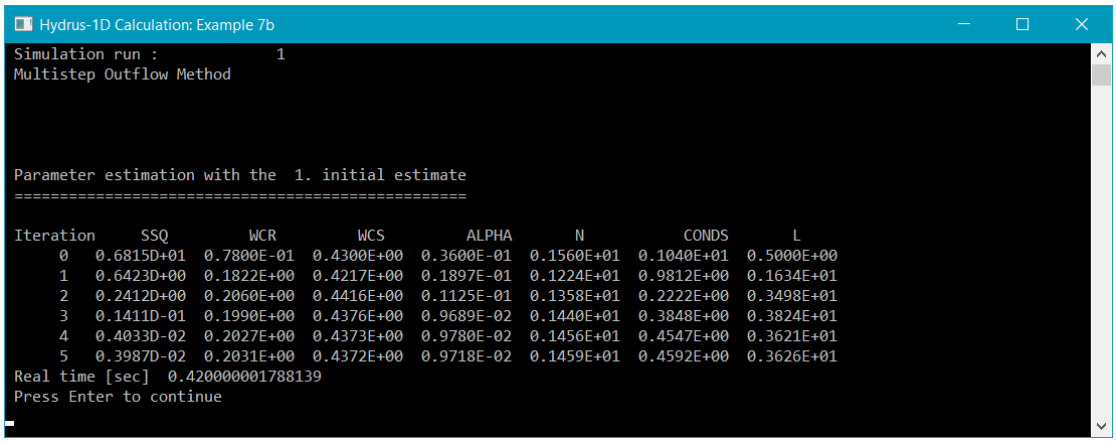

Figure 7b.1. The DOS window in which the inverse computational module h1d_clci.exe is executed.

This window shows selected information about the inverse run, such as the number of iterations (*Iteration*), the value of the objective function being minimized (*SSQ*), and values of optimized parameters at each inverse iteration. When the simulation ends, the Run Time in seconds is displayed. You are now asked to "*Press Enter to Continue*". Once the keyboard button "Enter" is pressed, the DOS window is closed, and the

program returns to the HYDRUS-1D GUI. Detailed output information about individual direct runs are not shown in the DOS window since we unchecked the "Screen Output" box in the Print Information dialogue window.

Post-Processing

Figure 7b.2 below compares the measured and optimized cumulative outflow curves for the soil sample (left) and measured and optimized pressure heads (right). Excellent agreement was obtained for both variables. The final fit had an R^2 of 0.9995. Table 7b.1 lists initial estimates and final values of the six optimized parameters.

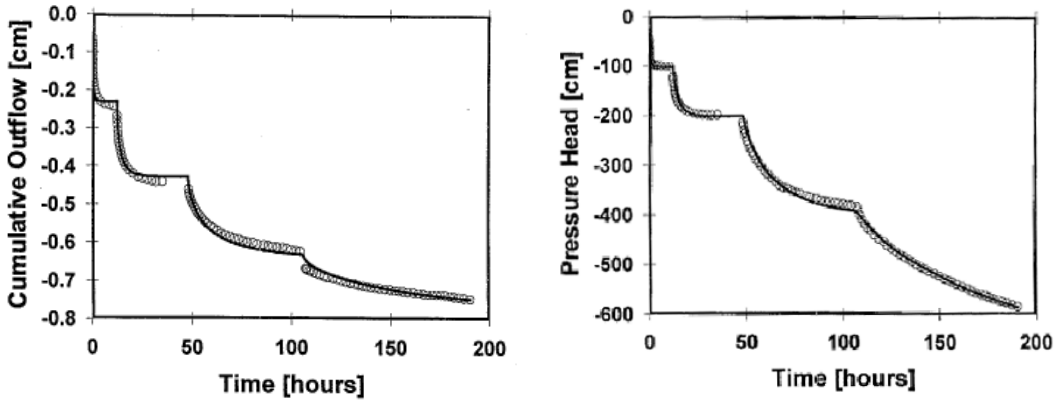

Figure 7b.2. Measured and optimized cumulative bottom flux (left) and pressure heads inside the soil sample (right) for a multistep outflow experiment.

Table 7b.1 Initial and final parameter values obtained for the multistep outflow experiment.

Parameter	Initial Estimate	Final Value
θ_r [cm³/cm³]	0.078	0.197
θ_s [cm³/cm³]	0.43	0.438
α [1/cm]	0.036	0.0101
n [-]	1.56	1.434
K_s [cm/h]	1.04	0.521
l [-]	0.5	3.80

Example 8: Heat Movement and Reactive Solute Transport

Example Description and Objectives

Example 8 simulates combined heat and solute transport through a 100-cm vertical uniform soil profile that maintains hydrostatic equilibrium conditions throughout the entire simulation. We further consider a stagnant boundary condition at the soil surface to account for volatile chemicals. The imposed upper 'Stagnant BC for Volatile Solutes' allows the diffusion of gas (oxygen in this case) from the atmosphere into the soil profile. The upper 'Temperature BC' allows the conduction of heat from the atmosphere to the soil profile that is initially at 20 ^{o}C. Diurnal temperature variations (daily cycles) are simulated using a sinus wave with an amplitude of 5 ^{o}C. The imposed initial and boundary conditions that result in no-flow conditions restrict heat and solute transport processes to be solely conductive and diffusive, respectively. Oxygen that diffuses into the soil profile is subsequently consumed via a first-order reaction process at a rate of 0.1 d^{-1} (the soil then consumes approximately 10% of the diffused gas per day).

Note that the standard HYDRUS module is intended mainly to simulate species for which the primary variable is the concentration in the liquid phase. Since molecular diffusion in the gaseous phase can be very dominant for volatile species, for which the majority of mass may be in the gaseous phase (e.g., oxygen, carbon dioxide), some restrictions on time steps or the numerical scheme (an implicit solution in this case) are required to achieve a stable numerical solution. Other HYDRUS modules, such as UnsatChem or HP1, in which the primary variable can be the concentration in the gas phase, have much more stable solutions.

Pre-Processing

Project Manager

- Select *Projects* Tab
- Button "New"
- Name: Example 7
- Description: Combined heat and solute transport
- *Button* "OK"
- Select *Example 8*
- Button "Open"

Main Processes

- Heading: Combined heat and solute transport
- Uncheck "Water Flow" (when water flow is unchecked, the initial condition and corresponding water content and fluxes will be constant during the simulation).
- Check "Solute Transport"
- Check "Heat Transport"
- *Button* "Next"

Geometry Information

- Leave as Default
- *Button* "Next"

Time Information

Time Discretization:

- Final Time (day): 4
- Maximum Time Step (day): 0.05 [refer to Appendix I.1 for explanation]
- Check Time-Variable Boundary Conditions
- Number of Time-Variable Records 1
- *Button* "Next"

Print Information

- Print Options: Leave as Default
- Number of Print Times: 3
- *Button* "Select Print Times"
- Print Times (day): 1, 1.5, 4
- *Button* "Next"

Iteration Criteria

- Leave as Default
- *Button* "Next"

Water Flow – Soil Hydraulic Model

- Leave as Default
- *Button* "Next"

Water Flow – Soil Hydraulic Parameters

- Soil Catalogue: Loam
- *Button* "Next"

Water Flow – Boundary Conditions

- Upper Boundary Condition: Atmospheric BC with Surface Runoff
- Lower Boundary Condition: Constant Pressure Head
- *Button* "Next"

Solute Transport

Time Weighting Scheme

- Check "Implicit Scheme"
- *Button* "Next"

Solute Transport Parameters

- Disp. = 5
- Diffus. W. = 1.7
- Diffus. G. = 17000
- *Button* "Next"

Solute Transport and Reaction Parameters – Solute 1

- $K_d = 0$
- Nu = 0
- Beta = 1.0
- Henry = 32
- SinkGas1 = 0.1

- *Button* “Next”

Solute Transport Boundary Conditions

- Upper Boundary Condition: Stagnant BC for Volatile Boundary
- Lower Boundary Condition: Zero Concentration Gradient
- Stagnant Boundary Layer: 1 cm
- Concentration in the Atmosphere: 0.3 mg/cm^3 [0.2 (an oxygen fraction in air) × 1.43 mg/cm^3 (the density of oxygen)]
- Initial conditions; Leave as Default
- *Button* “Next”

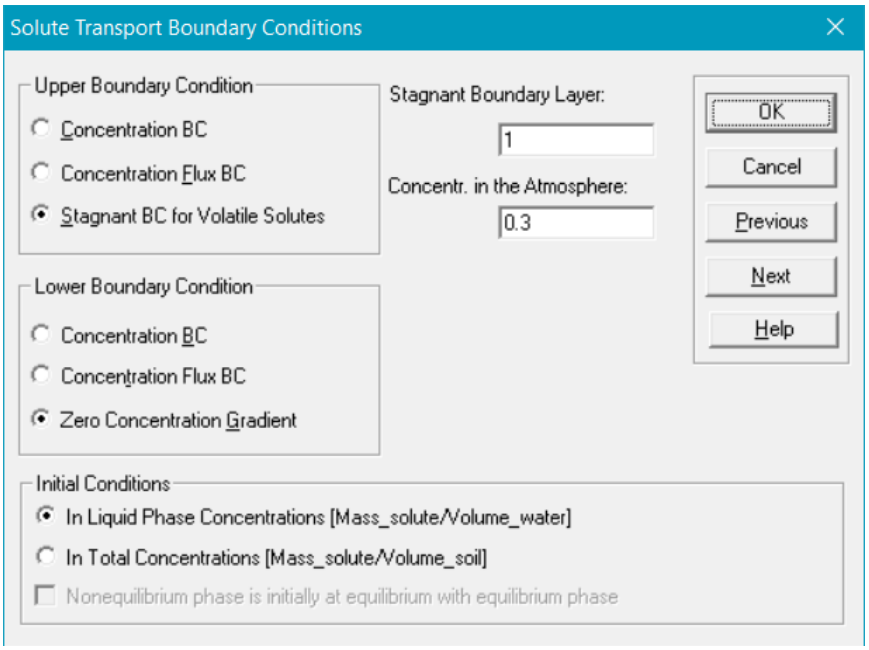

Figure 8.1. The **Solute Transport Boundary Conditions** dialog window.

Heat Transport Parameters

You must now select heat transport parameters using the dialogue window shown in Figure 8.2. Temperature fluctuations may either be explicitly provided as time-variable boundary conditions or may be simulated using a sinus wave having a specified amplitude and a time period. The latter is usually 1 day (or 1 year) thus simulating diurnal (or annual) temperature variations. Note that when the “Time-Variable Boundary Conditions” option is selected, the temperature amplitude is specified in the “Time-Variable Boundary Conditions” dialog window where different values can be specified on each record. When the soil textural class is selected (e.g., clay, loam, or sand), default heat transport parameters (b1, b2, and b3) are provided (in general in the units of [$WL^{-1}K^{-1}$; $MLT^{-3}K^{-1}$], but in this particular example in [kg cm d^{-3} K^{-1}]). Users should specify the volumetric fractions of solid (Solid) and organic matter (Org.M.), along with the longitudinal thermal dispersivity (Disp.). The units of the default values for the “Volumetric heat capacity” are in general in [$JL^{-3}K^{-1}$; $ML^{-1}T^{-2}K^{-1}$], except in this particular example where we use [kg/(cm.day^{2}K)] and hence larger numbers. Note that the mass units used for solute concentrations, the bulk density (and the distribution coefficient), or thermal parameters can be different.

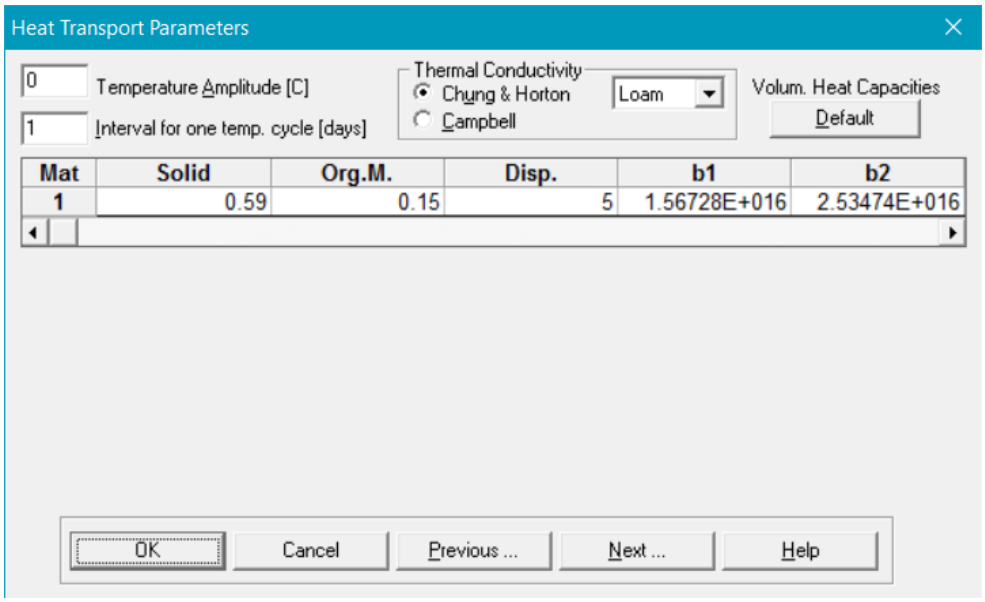

Figure 8.2. The **Heat Transport Parameters** dialog window.

- Temperature Amplitude (C): 0
- Interval for one temp. cycle (day): 1
- Thermal Conductivity: Select "Loam" (this will provide values for b1, b2, and b3)
- Volumetric Heat Capacities: *Button* Default (this will provide values for C_o, C_n, and C_w)
- Solid: 0.59
- Org.M.: 0.15
- Disp.: 5
- *Button* "Next"

Heat Transport Boundary Conditions

- Upper Boundary Condition: Temperature BC
- Lower Boundary Condition: Zero Gradient
- *Button* "Next"

Time-Variable Boundary Conditions

- Time (day): 4
- Precip. (cm/day): 0
- Evap. (cm/day): 0
- hCritA: 50000
- tTop (^{o}C): 30
- tBot (^{o}C): 20
- Ampl (^{o}C): 5
- cTop: 0 (not considered)
- cBot: 0 (not considered)

Soil Profile – Graphical Editor or Toolbar

- **Menu**: Conditions->Profile Discretization

- *Button* (on left-side Edit Bar) “Insert Fixed”: Select node at the 25-cm depth
- *Button* (on left-side Edit Bar) “Density”: Select surface node
- Nodal Density (Lower Density) = 0.1
- **Menu**: Conditions->Observation Points or **Toolbar** 
- *Button* (on left-side Edit Bar) “Insert”: Select nodes at depths 0 cm, 0.88 cm, and 25 cm
- **Menu**: Conditions->Initial Conditions->Pressure Head or **Toolbar** 
- *Button* (Edit Bar) “Edit Condition”: select with the Mouse the entire domain, left click
- Pressure Head Distribution: Top value = -100, Bottom value = 0, uncheck "Use top value for both"
- **Menu**: Conditions->Initial Conditions->Temperature (Leave as default 20^{o}C)
- **Menu**: Conditions->Initial Conditions->Concentration (Leave as default 0)
- *Button* “OK”
- **Menu**: File->Save Data or **Toolbar** 
- **Menu**: File->Exit

Soil Profile – Summary

- *Button* “Next”

Execute HYDRUS

- **Menu**: Calculation->Execute HYDRUS or a **Toolbar** button  .

Post-Processing

Observation Points

Figures 8.3 shows liquid concentrations of the diffused gas at depths of 0, 0.88 and 25 cm. Note that the concentration at the soil surface (0 depth) attains almost instantaneously the maximum (saturation) concentration of 0.009 mg/cm^3 (in equilibrium with the atmospheric gas concentration). This apparent artifact is a result of very fast molecular diffusion across a relatively narrow (0.5 cm) stagnant surface layer. Had a smaller initial time step been used, the surface concentration would have increased more gradually before reaching an equilibrium value. Note how the concentration at the very small depth of 0.88 cm starts from a smaller value (red line in Figure 8.3) and then gradually attains the saturation concentration. The transport of oxygen is slower in the soil due to tortuosity (restricted pore continuity) and retardation (equilibration between gaseous and liquid phases). After 4 days, the concentration at a depth of 25 cm does not yet reach the saturation limit.

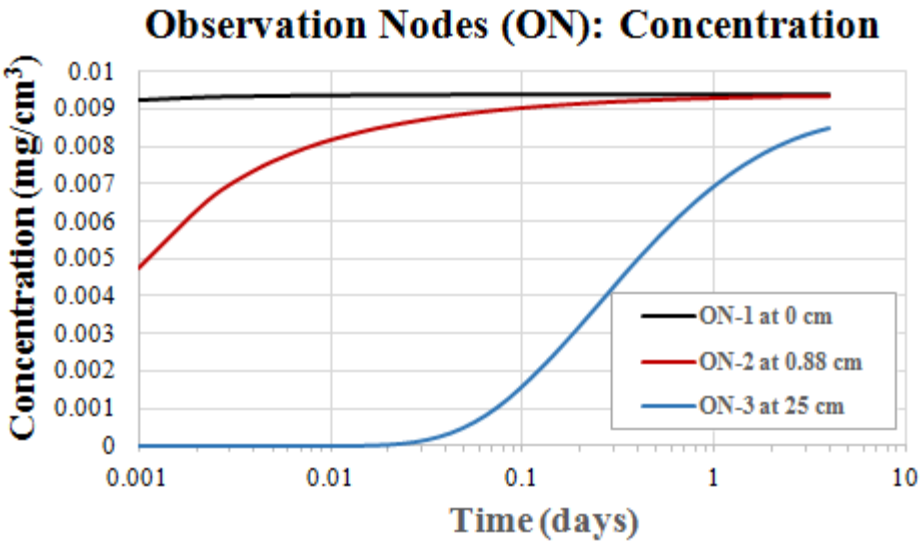

Figure 8.3. Solute concentrations at the soil surface and at depths of 0.88 and 25 cm.

Figure 8.4 shows the applied temperature boundary condition, which represents diurnal, day-night fluctuations (with temperatures of 30 ± 5 ^{o}C and maximum temperatures at 1 p.m.). The temperature at 25 cm starts increasing in response to the temperature gradient. Daily fluctuations are apparent also at a depth of 25 cm, albeit at a much lower amplitude. If the simulation were extended to much larger times, one could see that at depths larger than 60 cm the fluctuations gradually disappear.

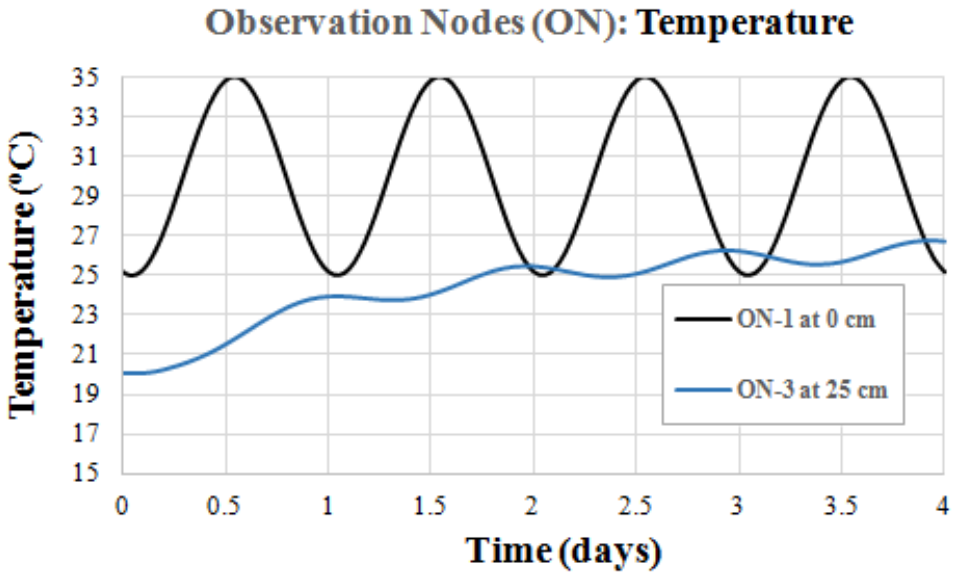

Figure 8.4. Temperatures at the soil surface and at a depth of 25 cm.

Profile Information

Figure 8.5 shows simulated liquid phase oxygen concentration profiles at different times. The downward advance of oxygen concentrations was mainly due to molecular diffusion in the air phase (note that the gaseous diffusion coefficient “Diff. G.” is about 10,000 times larger than the liquid phase diffusion coefficient "Diff. W."). This implies that the concentration advance always will be much faster in drier soils. Nevertheless, the concentration advance is the same in both gaseous and liquid phases due to the assumption of equilibrium partitioning between the two phases (the Henry's law).

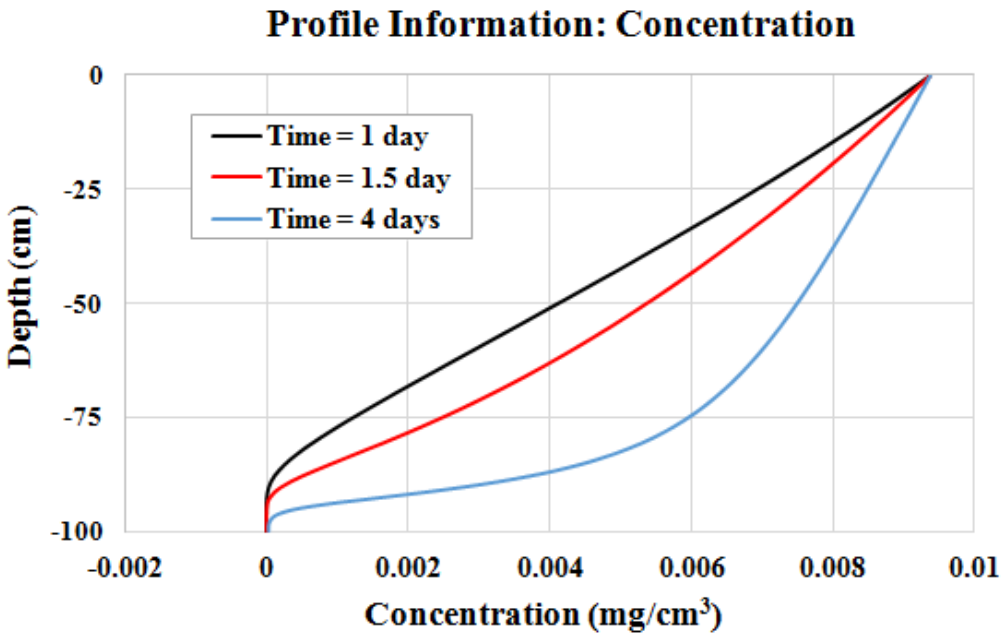

Figure 8.5. Liquid phase oxygen concentration profiles at different times.

Figure 8.6 shows the temperature profiles at various times. Note how the imposed boundary temperature (at the soil surface) fluctuates between 25 and 35 ^{o}C (30 ± 5 ^{o}C). At a depth of 100 cm, the temperature slowly increases above the initial 20^{o}C; if you were to extend the simulation to much larger times, a steady state situation equal to 30^{o}C would be reached (i.e., diurnal fluctuations do not affect the soil temperature at this depth).

Solute Fluxes

Figure 8.7 shows the cumulative solute fluxes, including the mass of oxygen diffused through the soil surface as well as the mass of oxygen consumed by the soil (the first-order reaction).

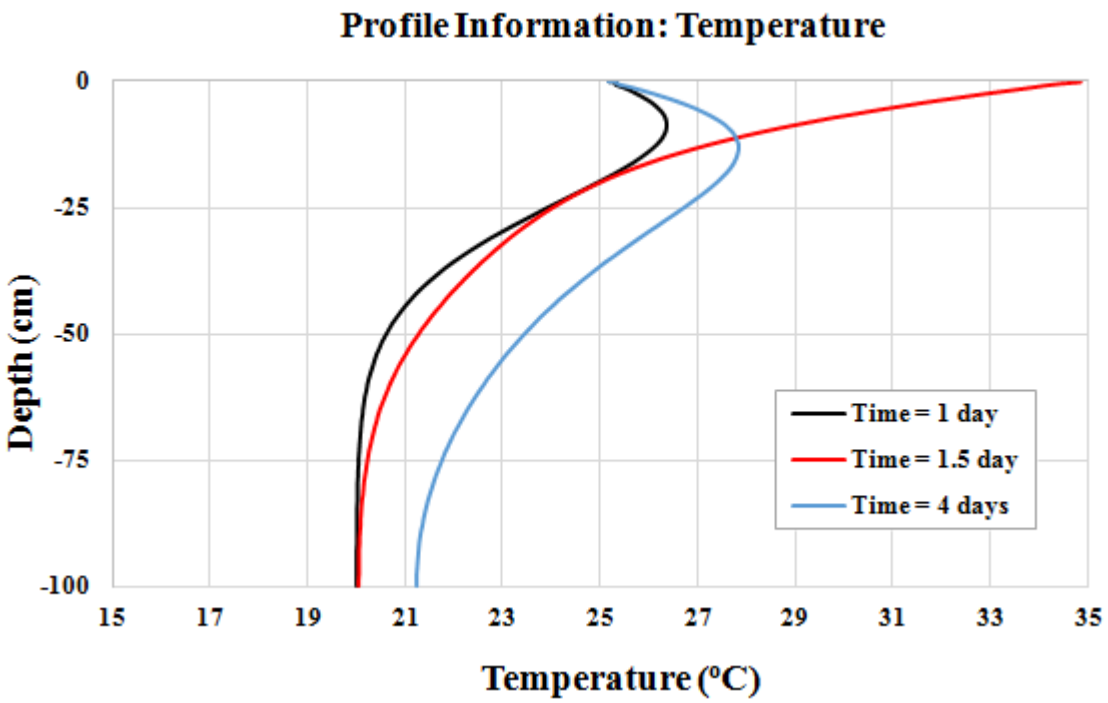

Figure 8.6. Temperature profiles at different times.

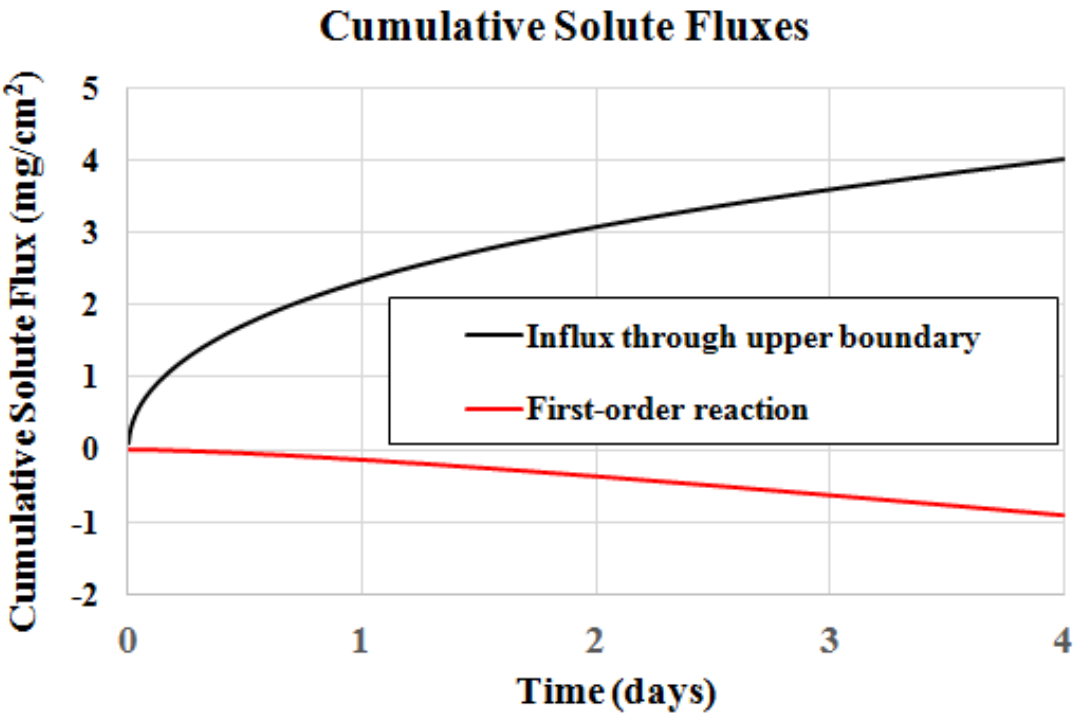

Figure 8.7. Cumulative solute fluxes.

Mass Balance Information

The mass balance information shown in Figure 8.8 refers to the following:

Length:	Depth of the soil profile
W-volume:	Total volume of soil water in the soil profile or selected subregions
In-flow:	Sum of fluxes flowing into and out of the soil profile (or subregions)
hMean:	Average pressure head in the soil profile (or subregions)
HeatVol:	Total heat energy stored in the soil profile
tMean:	Average temperature in the soil profile (or subregions)
ConcVol:	Total solute mass in the soil profile
cMean:	Mean concentration
Top Flux:	Flux into (at the top) the soil profile
Bot Flux:	Flux out of (at the bottom) the soil profile

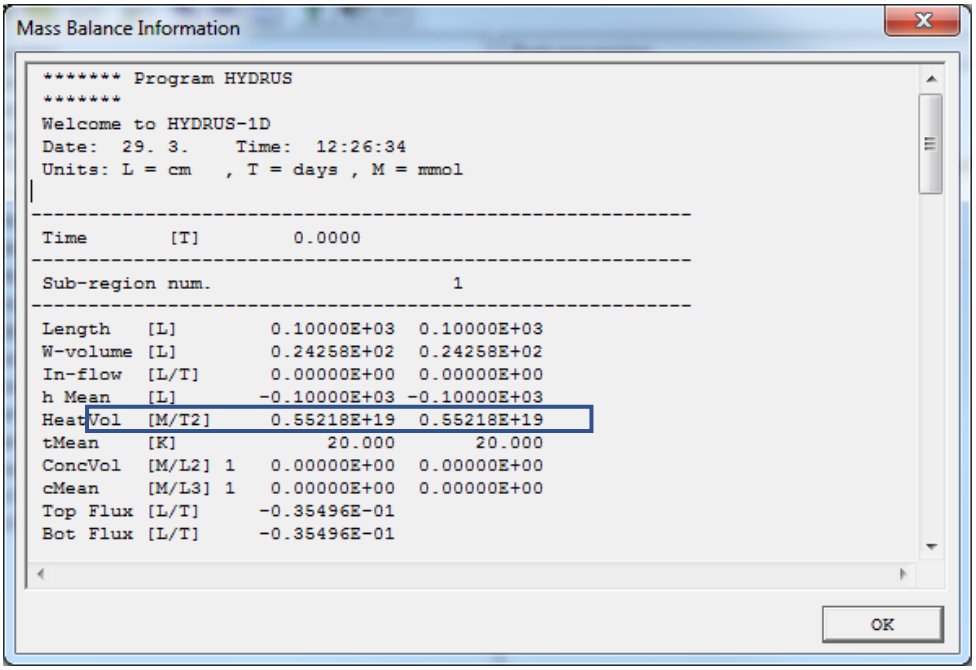

Figure 8.8. The mass balance information at Time=0.

Sample calculation for 'HeatVol' at the beginning of the simulation

Initial temp. = 20 ^{o}C = 293.15 K
Domain volume = 100×1×1 cm^3 (assuming a unit width and length in the horizontal directions)

Volumetric heat capacity of the solid phase, C_n = 1.433 × 10^{14} kg/(cm.day^{2}K)
Volumetric heat capacity of the organic matter, C_o = 1.874 × 10^{14} kg/(cm.day^{2}K)
Volumetric heat capacity of the liquid phase, C_w = 3.12 × 10^{14} kg/(cm.day^{2}K)
Solid fraction = 0.59
Organic matter fraction = 0.15
Water content = 0.243 (initial water content)

Total Volumetric Heat capacity, C_{soil} = (1.433×0.59 + 1.874×0.15 + 3.12×0.243) × 10^{14} = 1.88 × 10^{14} kg/(cm.day^{2}K)

Heat volume stored in the soil profile at initial time = Volumetric heat capacity × Soil volume × Temperature (=C_{soil} ×V_{soil} × T) = 1.88 × 10^{14} × 100 × 293.15 = 0.552 × 10^{19} kg.cm^2/day^2 = 0.552 × 10^{19} × 10^{-4} / (60×60×24)^2 = 73,945 kg.m^2/sec^2 (Joules)

Note that HYDRUS-1D reports this value for a one-dimensional soil profile, i.e., in kg/day^2 [MT^{-2}]. This value needs to be multiplied by the land surface area to obtain the heat storage in three dimensions.

Appendix I: Notes on Spatial and Temporal Discretization

Temporal Discretization

Four different time discretizations are used in HYDRUS-1D: (1) time discretizations associated with the numerical solution, (2) time discretizations associated with the implementation of boundary conditions, (3) time discretizations which provide printed output of the simulation results (e.g., nodal values of dependent variables, water, solute mass balance components, and other information about the flow regime), and (4) time discretizations associated with data defining the objective function in the inverse mode of HYDRUS-1D (e.g., measured water contents, pressure heads, concentrations, and/or water or solute fluxes). Discretizations 2, 3, and 4 are mutually independent; they generally involve variable time steps as described in the input data file. Discretization 1 starts with a prescribed initial time increment, Δt_{init}. The time increment, Δt, is automatically adjusted at each time level according to the following rules:

- Discretization 1 must coincide with time values resulting from time discretizations 2, 3, and 4.
- Time increments cannot become less than a preselected minimum time step, Δt_{min}, nor exceed a maximum time step, Δt_{max} (i.e., $\Delta t_{min} \leq \Delta t \leq \Delta t_{max}$).
- If, during a particular time step, the number of iterations necessary to reach convergence is ≤ 3 (It_{min}), the time increment for the next time step is increased by multiplying Δt by a predetermined constant >1 (k_1, usually between 1.1 and 1.5). If the number of iterations is ≥ 7 (It_{max}), Δt for the next time level is multiplied by a constant <1 (k_2, usually between 0.3 and 0.9).
- If, during a particular time step, the number of iterations at any time level becomes greater than a prescribed maximum (It_{crit}, usually between 10 and 50), the iterative process for that time level is terminated. The time step is subsequently reset to $\Delta t/3$, and the iterative process restarted.

Parameters Δt_{init}, Δt_{min}, Δt_{max}, It_{crit}, It_{min}, It_{max}, k_1, and k_2 are specified by a user at input. The recommended values for these parameters are as follows:

Parameter	Recommended value	Comment
Δt_{init}	1 s (15 minutes)	The recommended value for the initial time step depends on the type of simulation and boundary conditions used. When simulating a process that starts with a large initial pressure head or concentration gradient at a particular boundary (e.g., ponded infiltration or a sudden change in the boundary concentration), use a small value of the initial time step (e.g., 1 s). When simulating a long-term process with variable boundary conditions (e.g., seasonal or multiyear simulation), start with a larger time step (e.g., 15 min). This because this initial time step is used whenever time-variable boundary conditions significantly change. If needed (if there is no convergence for Δt_{init}), the program will still use a smaller time step than Δt_{init}, but starting with a larger Δt_{init} leads to more efficient calculations. In general, smaller initial time steps must be used for soils with more nonlinear soil hydraulic properties (e.g., coarse textured soils) and larger initial time steps can be used for soils with less nonlinear soil hydraulic properties (e.g., loam)
Δt_{min}	1 s	Always specify a small minimum allowed time step, on the order of 1 s. This value may never be used, but it provides the code with the flexibility when it may be needed, e.g., when there is a sudden change in boundary fluxes and HYDRUS-1D may not converge with larger time steps.
Δt_{max}	large	This is a relatively unimportant parameter, and a large value may be specified. Since HYDRUS-1D automatically selects its optimal time step, there is usually no need to constrain that. The only time when there is a need to constrain the time step is likely for cases when HYDRUS-1D is asked to generate internally intra-daily variations in temperature, or in evaporation and transpiration fluxes. Then there is a need to have time steps smaller (e.g., 1 h) so that these daily variations can be properly modeled.
It_{crit}	10	It is usually not helpful to use a larger value than 10. If HYDRUS-1D does not converge in 10 iterations, it is not likely that it will do so with more iterations. Even if it does, it is much more efficient to reduce the time step and attempt to find the solution with smaller time steps, which is done automatically by the program when It_{crit} is reached.
It_{min}	3	The optimal value in most cases.
It_{max}	7	The optimal value in most cases.
k_1	1.3	The optimal value in most cases. Only when there is a saturated zone in the profile, e.g., a perched water layer, the numerical solution may be more stable with smaller k_1 (e.g., 1.1).
k_2	0.7	The optimal value in most cases.

Spatial Discretization

The finite element mesh is constructed by dividing the soil profile into linear elements whose sizes are defined by the *z*-coordinates of the nodes that form the element sides. Finite element dimensions must be adjusted to a particular problem:

1. They should be made relatively small at locations where large hydraulic gradients are expected. This often happens close to the soil surface where highly variable meteorological factors can cause rapid changes in the soil water content and corresponding pressure heads. Similarly, regions with sharp gradients can be located in the vicinity of internal sources or at the interface of two contrasting soil types. Hence, we recommend using relatively small elements at and near the soil surface. The size of elements can gradually increase with depth to reflect the generally much slower changes in pressure heads at deeper depths. To decrease numerical errors, we also recommend using very similar sizes for neighboring elements. The ratio of the sizes of two neighboring elements is not recommended to exceed about 1.5.

2. The required size of finite elements close to the soil surface also depends very much on how boundary conditions are specified. When boundary conditions are specified for daily or shorter time intervals, they often involve short-duration fluxes of a large magnitude. The local spatial discretization needs then to be finer (on the order of cm or even less) than when boundary conditions are specified for longer time intervals (e.g., weekly or monthly).

3. The element dimensions should also depend upon the soil hydraulic properties. For example, coarse-textured soils having relatively high n and α values generally require a finer discretization than medium-textured soils. That is because the soil hydraulic functions of coarse-textured soils are more nonlinear and hence may cause less stable numerical solutions. This is reflected by sharper pressure head fronts for sandy soil profiles compared to medium- and many fine-textured soil profiles. Hence, we require more FE nodes to be able to describe the sharp moisture fronts in coarse-textured soils using elements on the order of 1 cm or less.

One generally cannot have finite elements for variably-saturated flow problems that are as large as for saturated problems (e.g., when using MODFLOW). While one can have large elements in the saturated zone (where the numerical solution is often based on the linear Boussinesq equation), one cannot have such elements in the unsaturated zone when the solution is based on the nonlinear Richards equation, especially close to the upper boundary where often sharp infiltration fronts are encountered (such as for infiltration into dry soils). The HYDRUS-1D model may be used to quickly figure out what discretization one can use for specific soil hydraulic properties and boundary conditions, and then use this discretization for two- or three-dimensional transport domains.

Appendix II. Boundary Conditions

Specifying appropriate boundary conditions (BCs) is one of the most critical tasks when constructing a numerical model. A water flow BC is usually represented by a known value of the water flux or the water pressure head along the outer boundary of the FE mesh. The external boundary of the selected flow domain provided the interface between the soil and the outside environment. A solute transport BC is usually represented by the solute concentration or the solute flux. Solving the governing equations for saturated/unsaturated flow/transport, which means finding new pressure heads and/or concentrations at each node of the FE mesh in a time-marching scheme, requires knowledge of the BCs. Otherwise the problem becomes mathematically not fully defined. The BCs in a model must simulate real-life conditions and hence must be selected with extreme care.

In HYDRUS-1D, boundary conditions are categorized as follows:

- System-dependent BCs: or dynamic BCs, meaning that they can change during the simulation (i.e., they depend on the solution at the end of each time step). They may depend on saturation conditions (as at a seepage face or a tile drain), and on soil hydraulic properties and/or climate conditions (as at the soil/atmosphere interface).

- System-independent BCs: This type of BCs is entirely known a priori, is implemented by the user, and is independent of the simulation results. System-independent water flow BCs include:
    - A known pressure head (as in Constant Pressure Head and Time-Variable Pressure Head BCs)
    - A known flux (as in No Flux, Constant Flux, Time-Variable Flux, and Deep Drainage BCs)
    - A known gradient (as in a Free Drainage BC)

Water Flow Boundary Conditions

In HYDRUS-1D, various water flow boundary conditions are selected as indicated in Figure II.1.

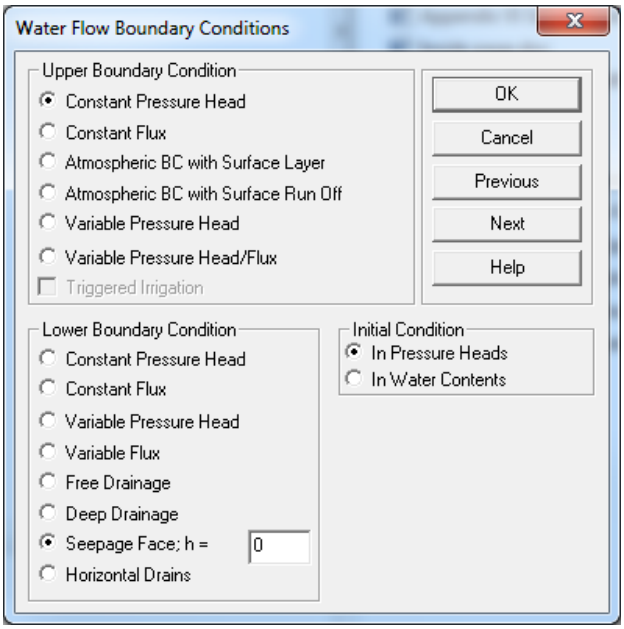

Figure II.1. The **Water Flow Boundary Conditions** dialogue window.

Constant Pressure Head BC

This BC refers to a constant pressure head during the entire simulation. Values of the pressure head (positive or negative) are entered as the initial pressure head for the uppermost node (for the upper BC) and/or the initial pressure head for the lowermost node (for the lower BC). This BC hence may be applied at the upper and lower boundaries of the model. Figure II.2 shows a variety of cases where a constant pressure head boundary condition is applicable:

- BC-1: A constant pressure head from a tension disc infiltrometer where the pressure head = h_1–h_2 (negative).
- BC-2, BC-3 and BC-4: Constant pressure heads from an overflowing tank, a Mariotte Bottle assembly, and a stream where the pressure head = *h* (positive).
- BC-5: A constant pressure head from a hanging water column where the pressure head = *h* (negative).

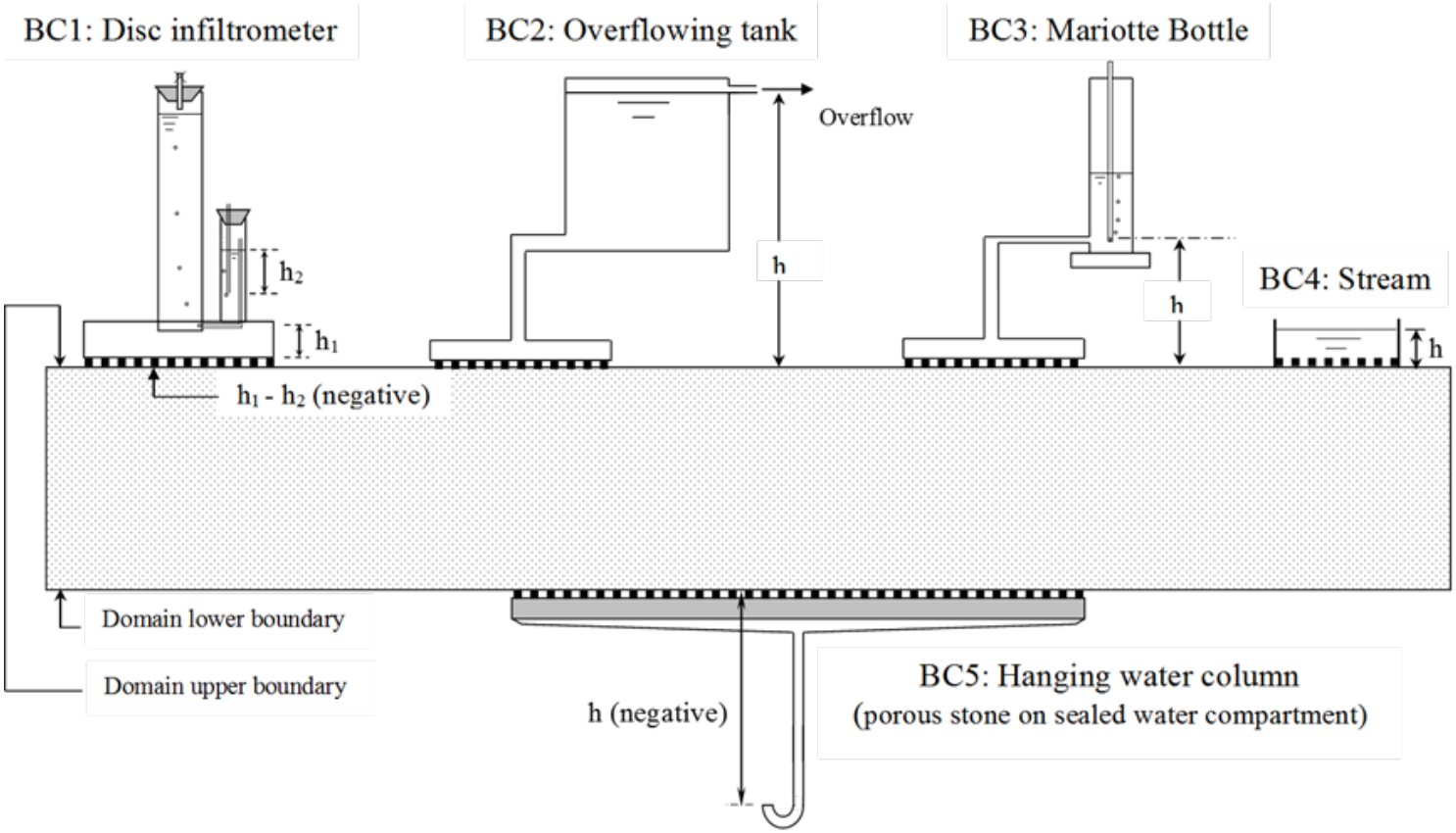

Figure II.2. Various applications for a constant head boundary condition.

Constant Flux BCs

This BC refers to a constant flux during the entire simulation. The flux (q) has the units of Length/time (L/T), similarly as the rainfall rate (cm/day). Fluxes are positive in the direction of the spatial coordinate (i.e., positive fluxes are upward for vertical flow or from left to right for horizontal flow, and vice versa, negative downward or from right to left). In the case shown in Figure II.3, the upper boundary flux is -1 cm/day (a downward influx into the domain) and the lower boundary flux is 1 cm/day (an upward influx into the domain).

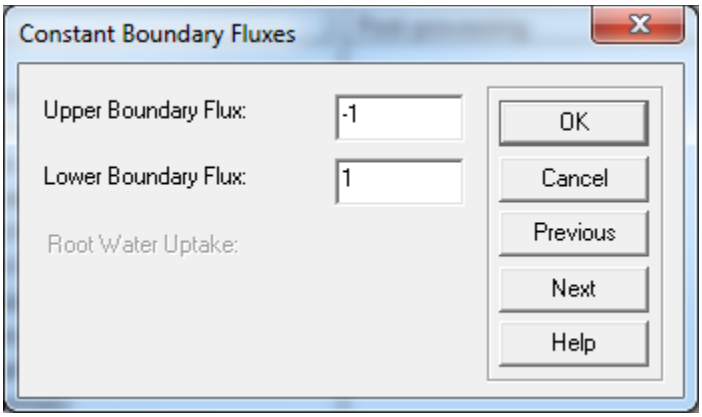

Figure II.3. The **Constant Boundary Fluxes** dialogue window.

Variable Pressure Head BCs

This BC refers to a time-variable pressure head that is entered as a time series. The time series has as many records as the number of times the pressure head changes at a boundary (one may enter as many records as required). For each record in the time series, the constant pressure head is effective during the period between the time of the previous record and the current one

To implement this BC, check the 'Time-Variable Boundary Conditions' check box in the 'Time Information' dialog window (Figure II.4) and enter 3 in the edit box 'Number of Time Variable Boundary Records'.

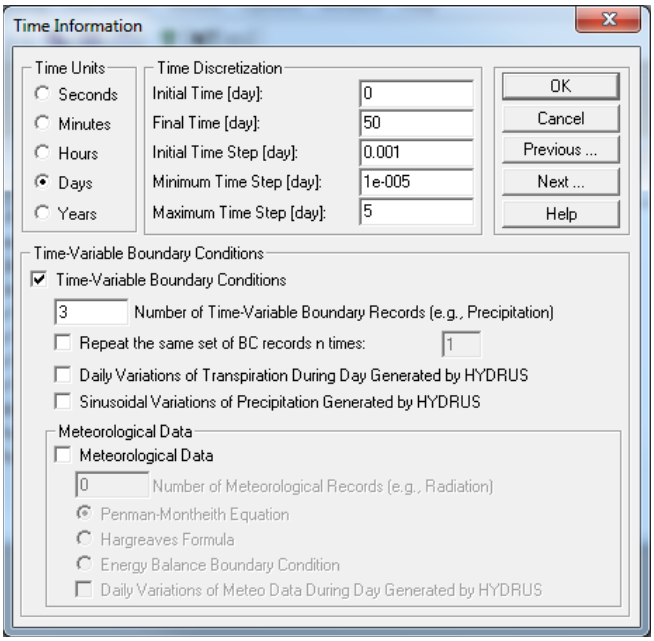

Figure II.4. The **Time Information** dialogue window.

Under 'Time-Variable Boundary Conditions' (Figure II.5), enter the Time and hTop (an applied pressure head):

i. 0 <Time ≤10 days, *h*=10 cm
ii. 10 <Time ≤25 days, *h*=0 cm
iii. 25 <Time ≤50 days, *h*=-30 cm

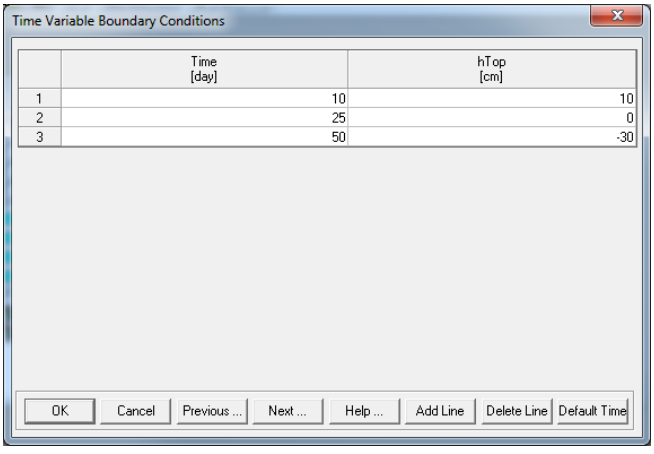

Figure II.5. The **Time Variable Boundary Conditions** dialogue window.

Variable Pressure Head/Flux BC

This BC refers to a time-variable flux that is entered as a time series. The data is then entered in a similar manner as the 'Variable Head' boundary condition, but instead of the pressure head (hTop) enter the boundary flux (FluxTop) in the time series (Figure II.6). An example is irrigation with a time-variable intensity.

To implement this BC, press the 'Time-Variable Boundary Conditions' check box in the 'Time Information' dialog window and enter 3 in the edit box 'Number of Time Variable Boundary Records'.

The variable 'KodTop' indicates whether a pressure head BC or a flux BC is used. KodTop =+1 indicates a pressure head BC and KodTop =-1 indicates a flux BC. In the case shown below, the BC at the soil surface is:

i. 0 <Time ≤ 10 days: the Pressure Head BC with *h*=10 cm
ii. 10 < Time ≤ 25 days: the Flux BC with a flux=-2 cm/day (influx at the surface)
iii. 25 < Time ≤ 50 days: The Pressure Head BC with *h*=-5 cm

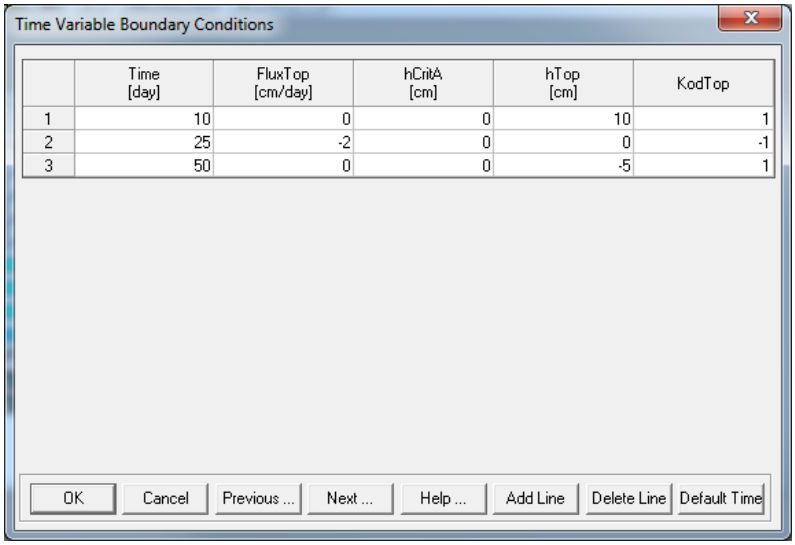

Figure II.6. The **Time Variable Boundary Conditions** dialogue window.

Atmospheric Boundary Condition

This boundary condition allows you to incorporate climatic conditions such as rainfall (precipitation), evaporation, and transpiration (root uptake) by plants. The latter is only activated if root water uptake is checked in the 'Main Processes' dialog window as in Figure II.7.

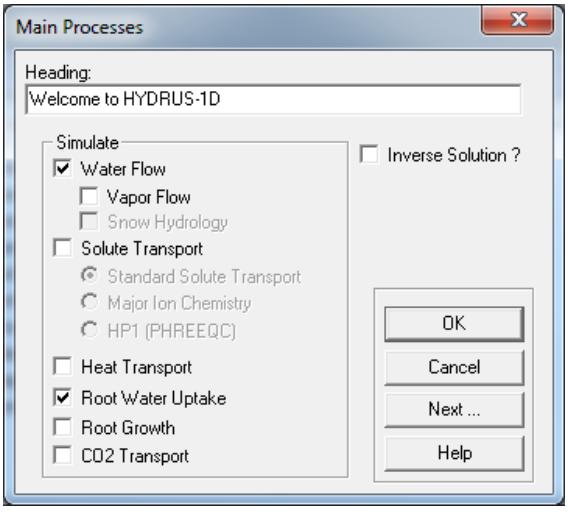

Figure II.7. The **Main Processes** dialogue window.

With this BC, you can control whether excess precipitation (i.e., when the precipitation rates exceed the saturated hydraulic conductivity of the soil surface) runs off instantly or ponds at the soil surface up to a certain height before it starts running off. When 'Atmospheric BC with Surface Layer' is checked, then you must specify the maximum pressure head allowed at the soil surface (Figure II.8). Once this pressure head (a thickness of the surface water layer) is reached water starts running off.

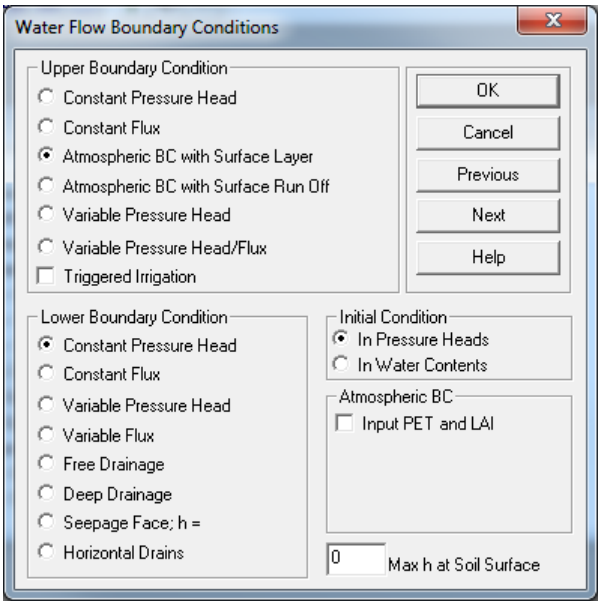

Figure II.8. The **Water Flow Boundary Conditions** dialogue window.

When an atmospheric flux boundary condition is used and the specified flux into the soil is higher than the infiltration capacity of the soil, HYDRUS-1D switches the BC from a flux BC to a pressure head BC. The pressure head at the boundary becomes zero when 'Atmospheric BC with Surface Run off' is checked and becomes equal to the thickness of the soil surface water layers (up to the 'Max h at Soil Surface' thickness) when 'Atmospheric BC with Surface Layer' is checked. The amount of water infiltrating across the soil surface is subsequently calculated according to the hydraulic conductivity and pressure head gradient at the soil surface (using Darcy-Buckingham's law), while excess water is instantly removed as surface runoff.

The window below appears only when 'Time-Variable Boundary Conditions' is checked in the 'Time Information' window. The data are then entered as a time series. The number of records in the series depends on the variability of the data, not the length of the simulation. For example, you may have a 5-day simulation where the precipitation is recorded at an average rate of 1 cm/day throughout the 5-day period, in which case you will need only one record as shown here (Figure II.9).

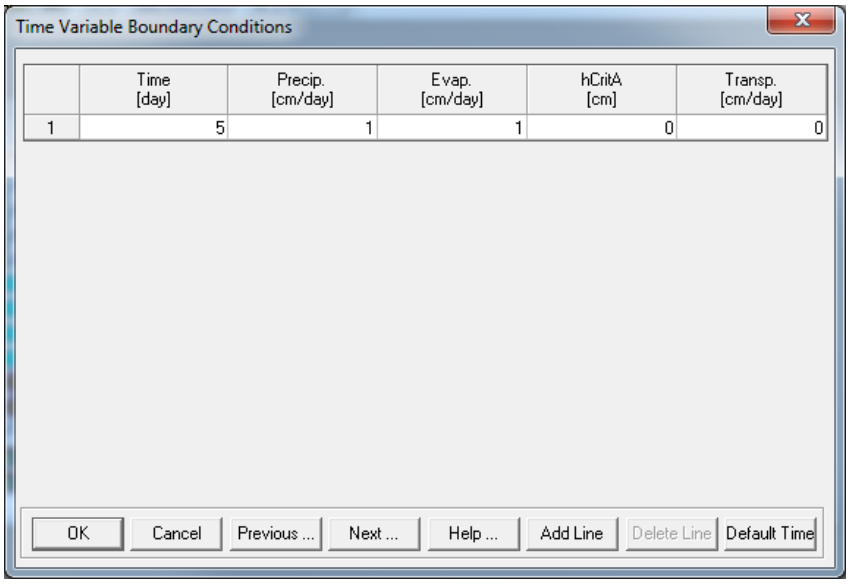

Figure II.9. The **Water Flow Boundary Conditions** dialogue window.

However, you may also have rainfall data obtained from a 0.5 mm tipping bucket for a 12-hour duration. The raw data are shown in columns 1 and 2 of Table II.2. Precipitation in HYDRUS-1D is entered as a rate (having the units chosen for the simulation, cm/day in this example). Using the tipping-bucket data, we must calculate a rate during each tipping period as follows (refer to Table II.2):

- Column 3: calculate the duration between consecutive tips. Convert 'min' to 'day' in Column 4.
- Column 5: convert rainfall to cm.
- Column 6: calculate cumulative time (simulation time).
- Column 7: calculate the rainfall rate (Column 5 / Column 4)
- Columns 6 and 7 are ready to be entered as 'Time Variable Boundary Conditions' under 'Time' and 'Precip.'.

In many cases (especially for very long simulations) the weather data are best entered from a spreadsheet. The easiest way to enter the data is as follows:

- Enter the exact number of Time-Variable Boundary Records (8 in this case).
- Open the 'Time-Variable Boundary Conditions' dialog window (Figure II.10) and copy the 8 cells from Columns 6 and 7 (shaded cells in Table II.2). The table should contain 8 rows. Select the first cell in Row 1 under column 'Time', and Press "Ctrl_v" on the keyboard; the data should appear as in the Window shown here.

Table II.2. Rainfall data.

Time	Rainfall (mm)	Duration (min)	Duration (day)	Rainfall (cm)	Time (day) Cumulative	Rate (cm/day)
5:36:00						
5:42:00	1	6	0.00417	0.1	0.0042	24
5:48:00	0.5	6	0.00417	0.05	0.0083	12
6:00:00	0.5	12	0.00833	0.05	0.0167	6
6:12:00	0.5	12	0.00833	0.05	0.0250	6
6:36:00	0.5	24	0.01667	0.05	0.0417	3
8:18:00	0.5	102	0.07083	0.05	0.1125	0.7059
14:00:00	0.5	342	0.23750	0.05	0.3500	0.2105
17:36:00	0.5	216	0.15000	0.05	0.5000	0.3333

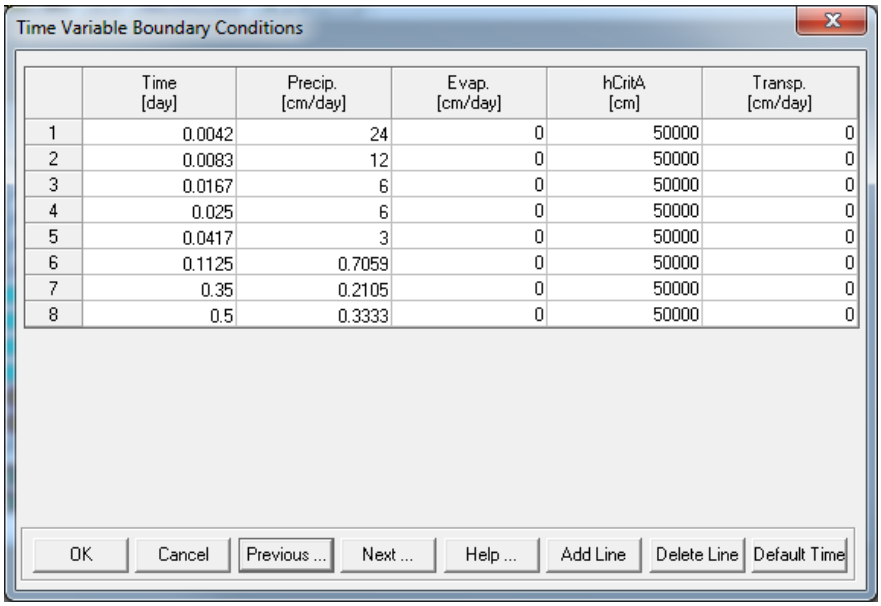

Figure II.10. The **Time Variable Boundary Conditions** dialogue window.

Triggered Irrigation

When this BC is selected, you can model 'Triggered Irrigation' whereby a constant flux (irrigation) is introduced to the soil surface when a certain pressure head is reached at a certain node (an Observation Node). To activate this option, check the 'Triggered Irrigation' box in the 'Water Flow Boundary Conditions' dialog window as shown below (Figure II.11).

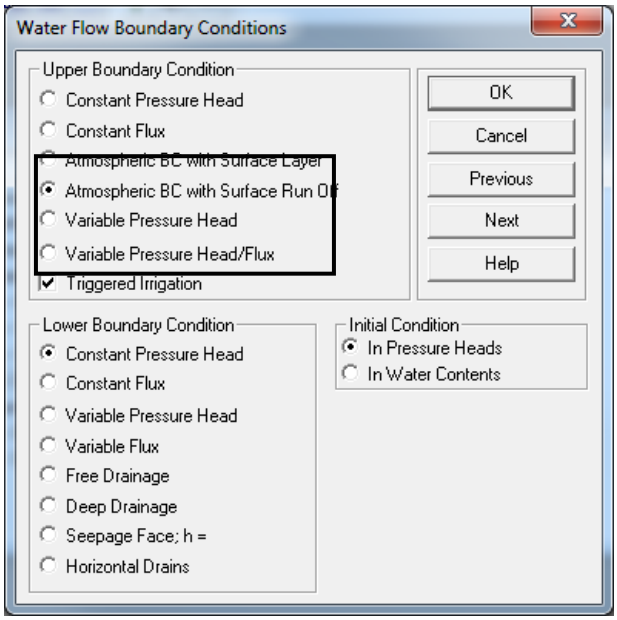

Figure II.11. The **Water Flow Boundary Conditions** dialogue window.

The required parameters are (Figure II.12):

- The number of the 'Observation point' triggering irrigation (the observation point should be specified in the Graphical Editor).
- The pressure head threshold at the observation point when irrigation is triggered.
- Irrigation rate, irrigation duration, and the lag time (the time interval between times when the pressure head triggering irrigation is reached and when irrigation starts).

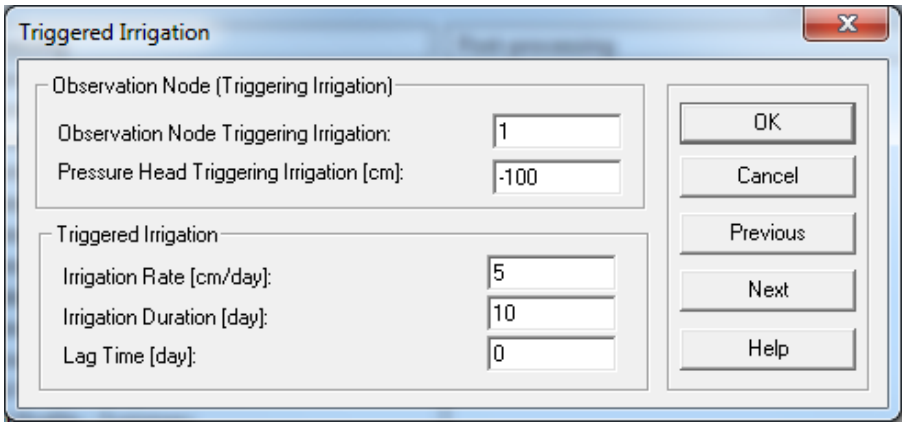

Figure II.12. The **Triggered Irrigation** dialogue window.

Free Drainage

This boundary condition specifies a unit total gradient at the lower boundary (outflow, drainage) of the soil profile. It is applicable for cases when the water table is located far below the domain of interest and thus does not affect flow in the transport domain. This BC assumes a unit total

vertical hydraulic gradient, that is, gravity flow with the pressure head gradient being zero. This boundary condition should be used only at the bottom of the domain.

Deep Drainage

This is a time-variable flux BC based on an observed experimental relationship between the pressure head at the bottom of the soil profile (usually positive) and discharge. Hence, it can only be used when such information is available. This BC relates flow at the bottom of the soil profile to the position of the groundwater table, which must be above the bottom of the soil profile (i.e., within the transport domain). The BC is based on an expression proposed by Ernst and Feddes (1979) (as reported by Hopmans and Stricker, 1989):

$$q = ae^{b|h-h_o|} \qquad \text{(II.1)}$$

where q is the discharge rate (or recharge rates), a and b are fitting parameters (obtained from experimental observations), h is the position of the groundwater level above the bottom of the soil profile, and h_0 is some equilibrium level of the groundwater table. The parameters a and b account for the effects of soil hydraulic properties (of the deeper layers), regional flow, and the position of the groundwater table on discharge.

The nodal flux at each time during the simulation is calculated using Equation II.1. This flux depends upon the pressure head, which varies during the simulation. Three values are required (Figure II.13):

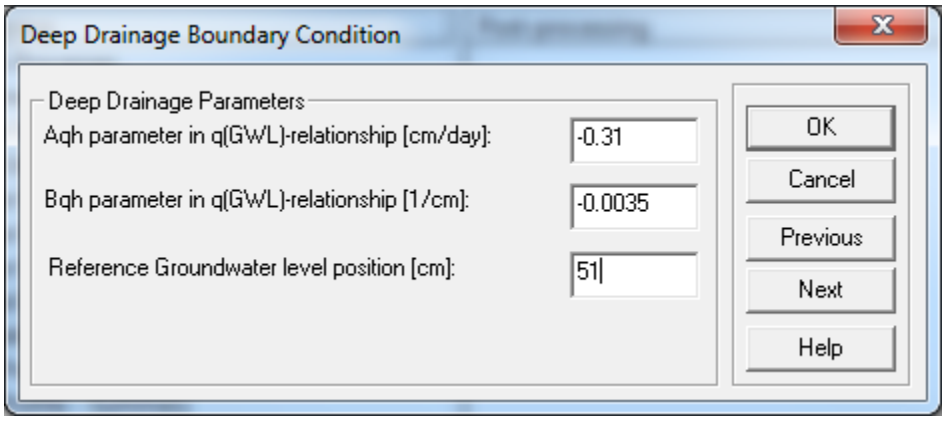

Figure II.13. The **Deep Drainage Boundary Conditions** dialogue window.

- The parameters '*a*' and '*b*' (of Equation II.1).
- The reference position of the groundwater table, which is like a datum value.

The calculated flux is assigned to the bottom node at each time step. Applications of this BC are limited because it requires field data to evaluate the fitting parameters. A recent example is given by Neto et al., 2016).

Seepage Face

This is a dynamic outflow (or drainage) BC that changes according to the flow conditions during a simulation. This BC is used at the bottom of lysimeters, laboratory soil columns, or tile drains where water freely drains through a soil surface exposed to the outer atmosphere. It only allows flow when saturation is attained, the pressure head at which saturation is achieved can be controlled (the default value is zero, Figure II.14).

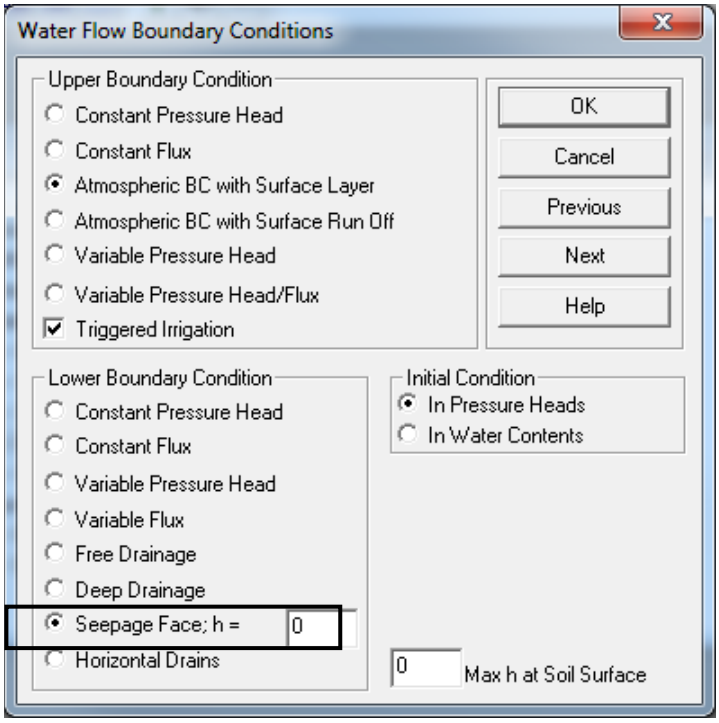

Figure II.14. The **Water Flow Boundary Conditions** dialogue window.

Solute Transport Boundary Conditions

Available solute transport boundary conditions include (Figure II.15):

- Concentration boundary conditions whereby users specify the liquid phase concentration at the boundary (for the upper and lower boundaries)
- Concentration flux boundary conditions whereby users specify the concentration of the infiltrating water (for upper and lower boundaries)
- A stagnant boundary layer for volatile solutes (applicable to the upper boundary)
- Zero concentration gradient (free drainage) (for the lower boundary)

Third-type (Cauchy or solute flux) boundary conditions prescribe solute fluxes across (not concentrations at) a boundary. Due to mixing with water (and solute) initially present in the profile, one will not get immediately the input ($C_{0)}$ concentration on the boundary. Since one prescribes a solute flux, one has complete control over the mass balance and how much solute enters into the transport domain.

When a first-type (Dirichlet or concentration) boundary condition is used, one prescribes the concentration at the boundary (not the flux into the domain). Since solute flux consists of two components, i.e., advective and dispersive fluxes, both of these are active on the boundary at the same time. Initially, there is a large concentration gradient, and thus the dispersive solute flux can be very large. In this case, one has a much larger flux into the domain than if one uses the third-type solute flux boundary condition.

We recommend using always a third-type boundary condition since that condition is physically the most realistic. Dirichlet conditions in most cases do not provide a conserve mass and hence do not provide a good alternative. You should use a Dirichlet condition only if, for example, a large reservoir of contaminant is in contact with the transport domain, in which case one can assume that the boundary concentration is fixed (e.g., for upward flow from a water table with groundwater having a certain concentration). Several have reviewed the implications of using different boundary conditions for various experimental conditions (e.g., van Genuchten and Parker, 1984; Skaggs and Leij, 2002)

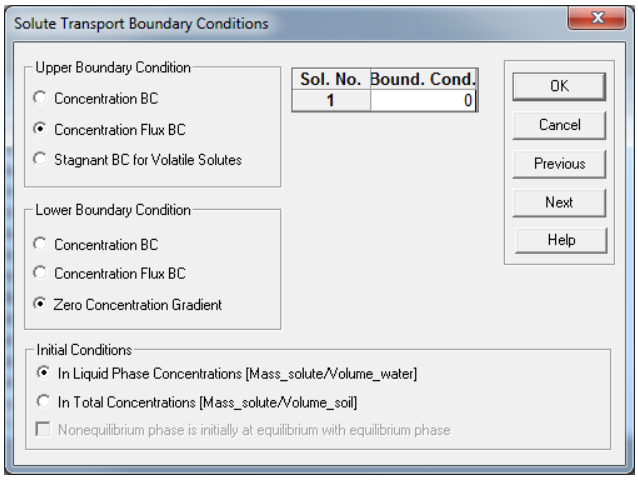

Figure II.15. The **Water Flow Boundary Conditions** dialogue window.

Appendix III: Unsaturated Soil Hydraulic Properties

Water Retention Properties

The fundamental relationship between the soil water content (usually calculated on a volumetric basis) and the pressure head (or the matric suction) is referred to as the soil-water retention curve (SWRC) or the soil water characteristic curve. The matric suction is the difference between the pore air pressure head and the pore water pressure head. If a change in the water content occurs at any point in a mass of soil initially in an equilibrium state, the soil matric suction (or the negative pore water pressure) at that point changes (assuming atmospheric conditions, the pore air pressure has a value of 0). Following this change, there will be a difference in the energy level between the point where the change occurred and the surrounding soil, which will cause water to flow into the soil until new equilibrium conditions are established (Croney, 1952). Knowledge of the water retention curve is essential when investigating how soil moisture reacts in response to changes in the pressure head, resulting from events such as infiltration, evaporation, and drainage. Due to the hysteretic behavior of soils with respect to wetting and drying processes, different SWRC curves may be obtained depending upon whether the soil is undergoing a drying cycle, a wetting cycle, or a re-drying cycle (Collis-George, 1955).

Shape of the Soil-Water Retention Curve

The general shape of the SWRC under wetting and drying conditions is shown in Figure III.1 on a semi-log scale. The following parameters are identified:

- The saturated volumetric water content, θ_s, which theoretically corresponds to the soil's porosity, but practically is often about 10-25% less because of dissolved and/or entrapped air.
- The air-entry value, *AEV*, is a critical value of suction, at which the largest pores in the soil matrix start losing water.
- The residual water content, θ_r, is the water content beyond which a further increase in the soil's suction results in only marginal changes in the water content.
- At very high suctions (negative pressure heads), the water content eventually becomes zero. This value is about 10^6 kPa (10^7 cm) and has been supported experimentally (e.g., Croney and Coleman, 1961; Koorevaar et al., 1983), as well as by thermodynamic considerations (Richards, 1965).

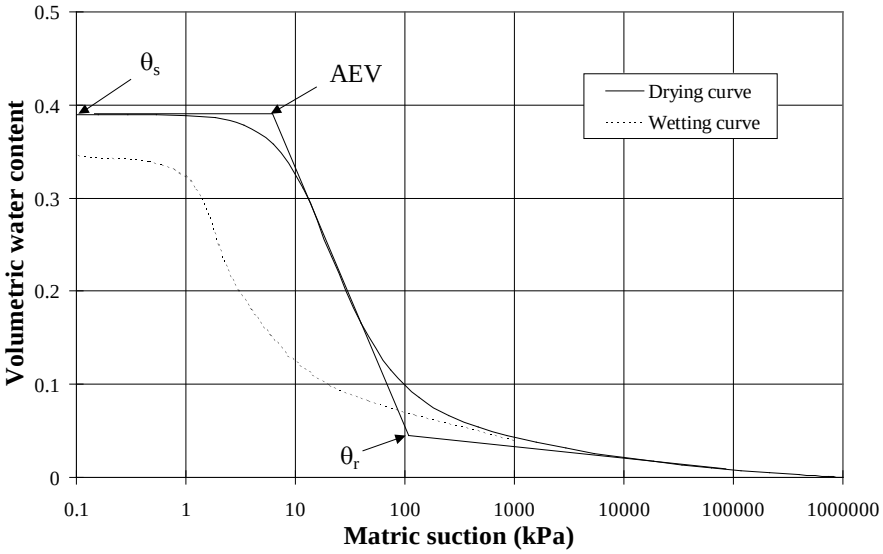

Figure III.1. The typical shape of a soil water retention curve.

The residual water content (θ_r) and the corresponding suction, sometimes termed the residual suction, have been defined in a number of ways in the literature. However, the accepted use of these terms is not always agreed upon. Tinjum et al. (1997) defined it as the water content corresponding to the asymptote of the SWRC at low degrees of saturation. van Genuchten (1980) defined θ_r as the water content at which its rate of change with respect to suction becomes zero, or when the liquid flow of water ceases (excluding the region near saturation).

Classically, moisture in the unsaturated zone is separated into three components: gravitational, pellicular, and hygroscopic water (e.g., Everett, 1993). Gravitational water is the moisture in a soil that can be drained by gravitational forces. Pellicular water is moisture in a soil that cannot be drained by gravity forces but can be lost by evaporation. Finally, the hygroscopic water is moisture that will never be lost through the above natural forces. The residual water content may be viewed as the water content at the limit of liquid water extraction. De-saturation beyond residual conditions occurs primarily as a result of vapor flow up to the point where the soil water content is in equilibrium with the vapor pressure of its surrounding. Brooks and Corey (1966) pointed out that it is difficult to determine the residual saturation of clayey materials; they related the residual saturation to the clay content of the soil. The well-defined, residual state for sands, silts, and their mixtures can reasonably well be predicted from the SWRC as shown in Figure III.1.

Models Describing the SWRC

A mathematical representation of the SWRC is essential when using numerical models for simulating fluid flow and mass transfer in the unsaturated zone. HYDRUS-1D allows users to select from five analytical models to describe the soil hydraulic properties: van Genuchten (1980), modified van Genuchten (Vogel and Cislerova, 1988), Brooks and Corey (1964), Kosugi (1996), and Durner (1994). The first three of these models are described briefly in the following section.

van Genuchten (VG) Model

van Genuchten (1980) proposed a mathematical representation of the SWRC, which depicts an S-shaped curve when plotted on a semi-log scale. His equation is given by:

$$S_e = \left(1 + \left|\alpha h\right|^n\right)^{-m} \qquad \text{(III.1)}$$

where α, m, and n are mostly semi-empirical fitting parameters (usually m=1-1/n), h is the pressure head, and S_e is the normalized volumetric water content (often referred to as effective saturation):

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \qquad \text{(III.2)}$$

in which θ is the volumetric water content at pressure head h, and θ_s and θ_r are the saturated and residual water contents, respectively.

Each of the three fitting parameters (α, m, and n) control part of the S-shape curve. Figure III.2 shows the effect of α (Alpha), which is closely related to the reciprocal of the air-entry value (AEV) of a soil. Coarse-grained soils have a low AEV and a high α value, whereas fine-textured soils have a lower α.

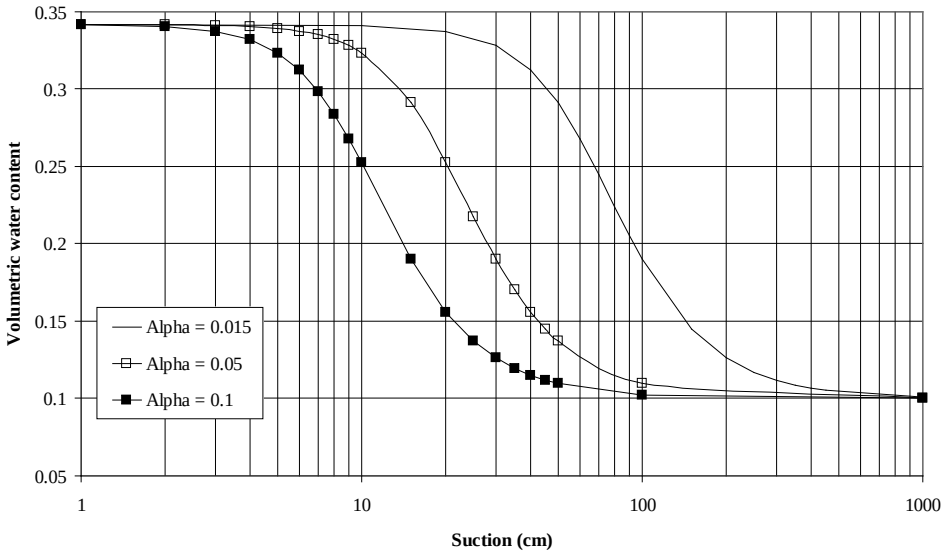

Figure III.2. The effect of α in the van Genuchten model on the SWRC.

Figure III.3 shows the effect of the n parameter, which controls the slope of the curve and reflects the width of the particle size distribution. The plot indicates that a unit increase in suction at or near the steepest part of the curve causes more water to be extracted from coarse-textured soils (high n) than from fine-textured soils (low n), but not at other places of the curve.

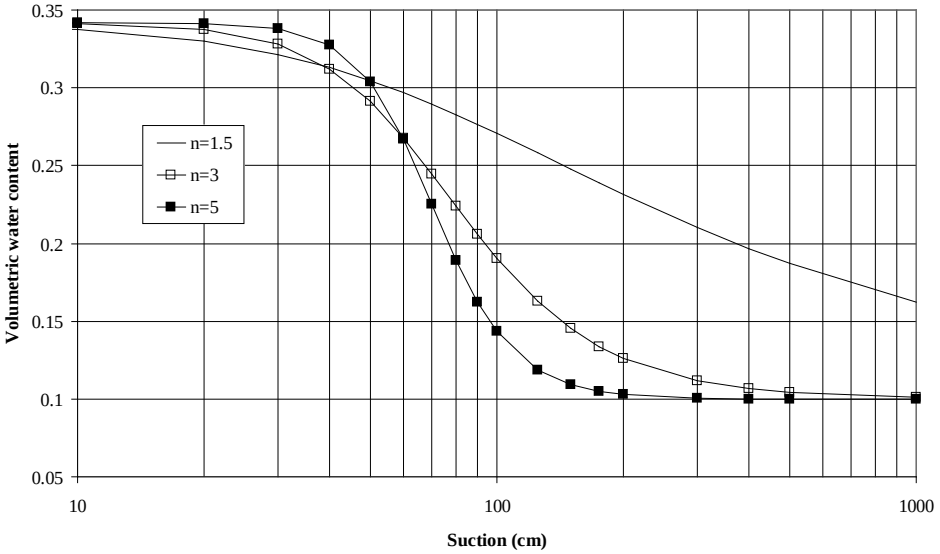

Figure III.3. The effect of *n* in the van Genuchten model on the SWRC.

When the parameters *n* and *m* are correlated (as when *m*=1-1/*n*), a relatively simple equation can be derived for the hydraulic conductivity function, *K*(*h*), when the retention function is combined with the theoretical pore-size distribution model of Mualem (1976) for *K* (see below). Figure III.4 shows that when the two parameters are correlated, the curvatures (A and B) of the S-shape curve become correlated. When individual values are assigned to *n* and *m* the curvatures in the wet and dry regions of the retention curve become independent (van Genuchten and Nielsen, 1985).

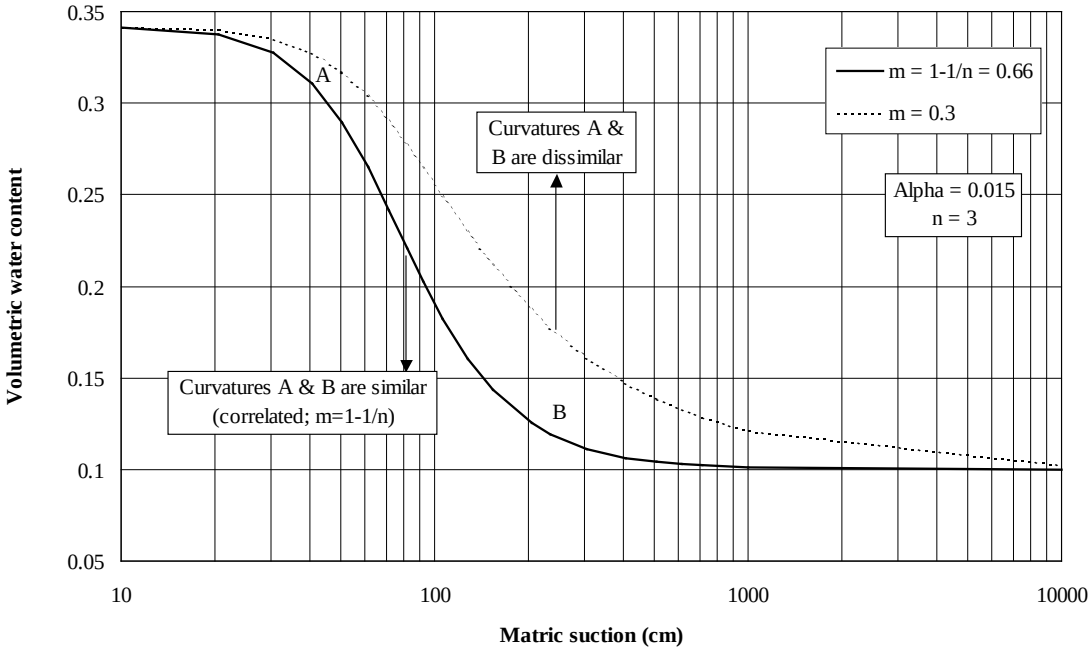

Figure III.4. The relation of *m* and *n* in the van Genuchten model.

van Genuchten Model with AEV of -2 cm

The unsaturated soil hydraulic properties are often described using the Mualem–van Genuchten (MVG) type analytical functions (van Genuchten, 1980). Recent studies suggest several shortcomings of these functions near saturation, notably the lack of the second-order continuity of the soil water retention function at saturation and the inability of the hydraulic conductivity function to account for macroporosity. Vogel et al. (1985) and Schaap and van Genuchten (2006) showed that a modified MVG formulation with a small but constant air-entry pressure in the water retention curve substantially improves the description of the hydraulic conductivity near saturation. It is thus recommended, especially for fine-textured soils with small values of the n parameter (n < 1.1-1.2), to use a modified van Genuchten-Mualem model with an air-entry value of -2 cm. In addition to improving the description of the hydraulic conductivity function, this modified MVG model also dramatically improves the convergence of the numerical solution.

The van Genuchten (VG) model that implements a small non-zero air-entry value (AEV) of -2 cm shows almost no effect on the macroscopic description of the water retention function of fine-textured soils compared to the original VG formulation. Selecting this option will introduce a small correction (like an air-entry value) in the water retention function to force the slope of the retention function ($d\theta/dh$) to become zero when approaching saturation at h=0 (see Figure III.5; note that the water content remains at saturation for suctions below 2 cm).

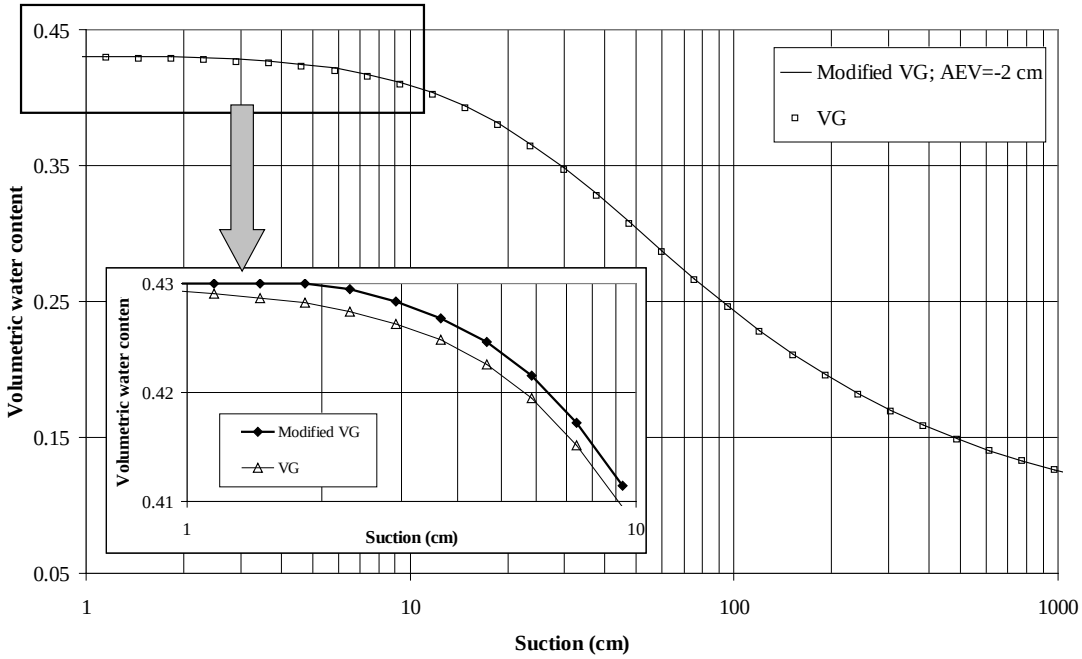

Figure III.5. The van Genuchten model with AEV of –2 cm.

We will show later that implementing this low non-zero AEV has a significant effect on the hydraulic conductivity function. This option is recommended for fine-textured soils (e.g., silty clays and clays), but should not be used for medium-, and especially coarse-textured, soils when the value of the parameter α becomes relatively large (say >0.02 or 0.05 cm). This rule applies

unless *n* is again less than about 1.1 or 1.2, which generally is not the case for medium- and coarse-textured soils. The -2 cm AEV should then be avoided since it introduces a Brooks and Corey (1964) type air-entry correction into the retention function to make the function less accurate for many soils (Schaap and van Genuchten, 2006).

Modified van Genuchten Model (Vogel and Cislerova)

Vogel and Cislerova (1988) modified the van Genuchten model by incorporating a non-zero AEV into the model. The modification was implemented by introducing a fictitious water content θ_m that is higher than θ_s and replaces θ_s in the van Genuchten model. This fictitious water content is used only when h<AEV. Above AEV the water content is equal to θ_s. Their retention model is given by

$$\theta = \begin{cases} \theta_a + \dfrac{\theta_m - \theta_a}{\left(1+\left|\alpha h\right|^n\right)^m} & h < AEV \\ \theta_s & h \geq AEV \end{cases} \qquad \text{(III.3)}$$

Figure III.6 shows how the model is implemented. The data points at suctions <17 cm are only a hypothetical continuation to the S-shape curve. That is, when the pressure head is below this value, the water content is fixed at θ_s.

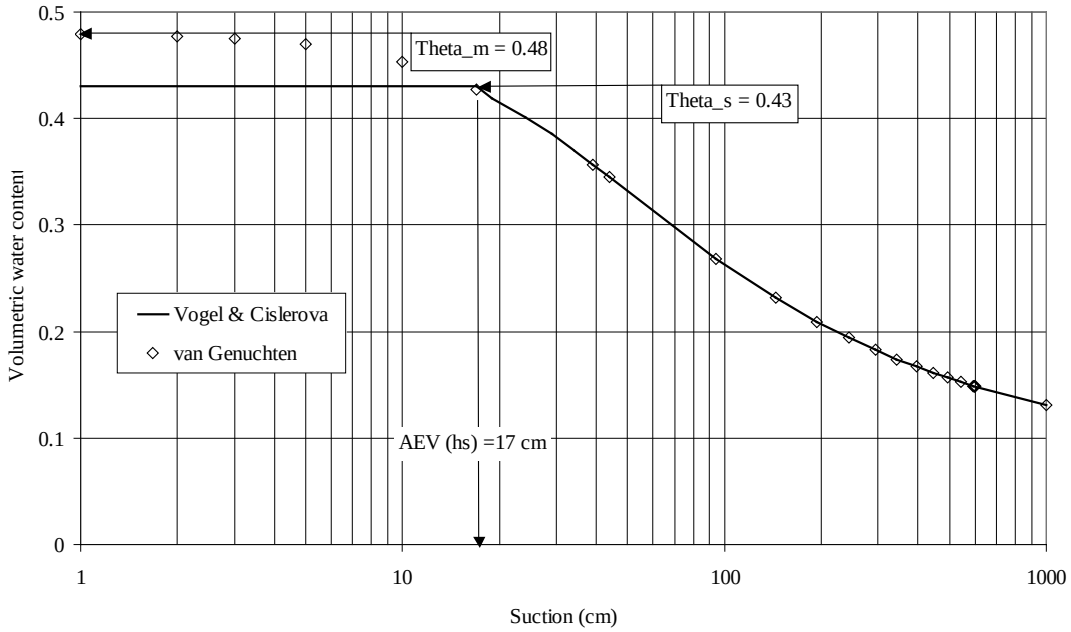

Figure III.6. The modified van Genuchten model.

Brooks and Corey (BC) Model

Brooks and Corey (1964, 1966) concluded from comparisons of a large number of experimental data that the SWRC could be described by the following formula:
given by

$$S_e = \left(\frac{AEV}{h} \right)^n \qquad \text{(III.4)}$$

where *AEV* is the air entry value (corresponds to $1/\alpha$ in the HYDRUS-1D GUI), and *n* is a soil characteristic parameter, called the pore-size-distribution index. Experimental data of suction and water content are often plotted as $\log|h|$ versus $\log \theta$. Linear regression can then be performed on the straight-line relationship. The slope and intercept of the best-fit line then correspond to $1/n$ and *AEV*, respectively. Figure III.7 shows a comparison of the BC model with the VG model using the parameters listed in Table III.1.

When using the Brooks and Corey functions in HYDRUS-1D, we recommended to either disable the internal interpolation tables or to set the lower limit above the air-entry value.

Table III.1. Parameters for two SWRCs in Figure III.7.

	θ_r	θ_s	α	n
van Genuchten	0.078	0.43	0.036	1.56
Brooks & Corey	0.027	0.434	0.0897	0.293

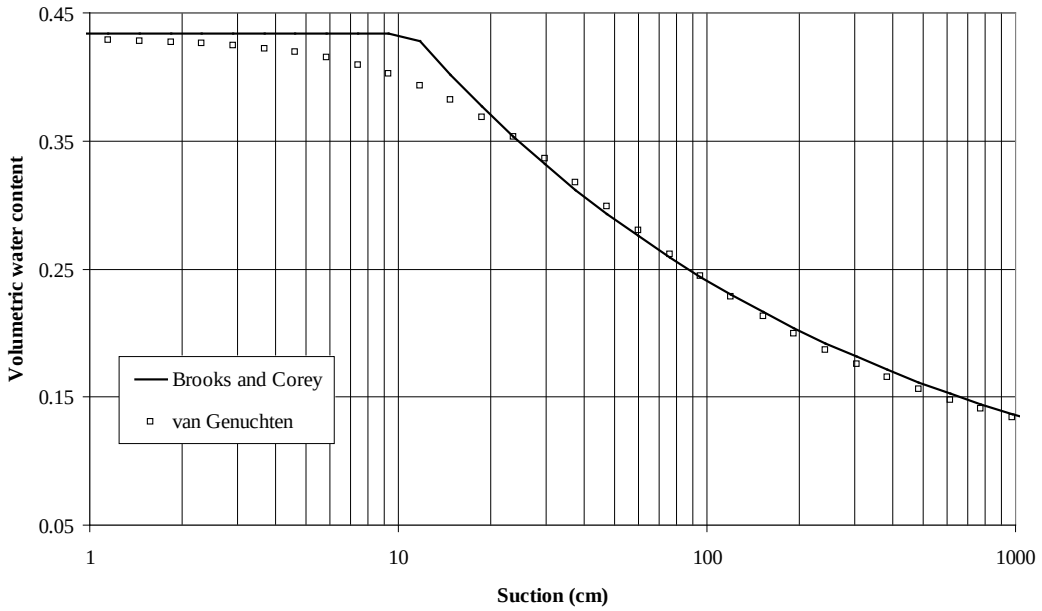

Figure III.7. Comparison of the Brooks and Corey and van Genuchten models.

Hydraulic Conductivity Functions

van Genuchten-Mualem Model

Mualem (1976) developed the following equation for predicting the relative hydraulic conductivity K_r from the knowledge of the SWRC:

$$K_r = S_e^{\,l} \int_0^{S_e} h^{-1}(\tau)d\tau \Big/ \int_0^1 h^{-1}(\tau)d\tau \qquad \text{(III.5)}$$

where h is the pressure head, given as a function of the dimensionless water content Se defined by Equation (III.2).

For the special case where m=1-1/n (the fitting parameters of Equation (III.1)), a closed-form solution was obtained by van Genuchten (1980) as follows:

$$K(h) = K_s S_e^{\,l}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \qquad \text{(III.6)}$$

where l is a pore connectivity parameter established to be 0.5 by Mualem (1976) and -1 by Schaap and Leij (2000). Equation (III.6) in combination with the VG retention model has been used successfully in an extremely large number of studies. They are the default functions in HYDRUS-1D.

van Genuchten Model with AEV of -2 cm

Choosing the approach by Vogel and Cislerova (1988) for the retention function substantially changes the shape of the predicted hydraulic conduction function, $K(h)$, based on Equation (III.5), as compared to the curve predicted using the standard VGM statistical pore-size distribution model (Vogel et al., 2001). The predicted $K(h)$ curve is then far less nonlinear and much more accurate for fine-textured soils (typically clays and silty clays). Using this option may also result in fewer numerical problems when modelling ponded infiltration or other variably-saturated flow problems. The -2 cm correction was first suggested by Vogel and Cislerová (1988) and worked out further by Vogel et al. (2001). Schaap et al. (2006) later showed that a -4 cm correction would be slightly better than -2 cm, but the difference is minimal.

Figure III.8 shows the impact of using this option. Note that the hydraulic conductivity functions are usually plotted on the log-log scale, but in this case we chose to plot it on a semi-log scale to emphasize the dramatic differences near saturation.

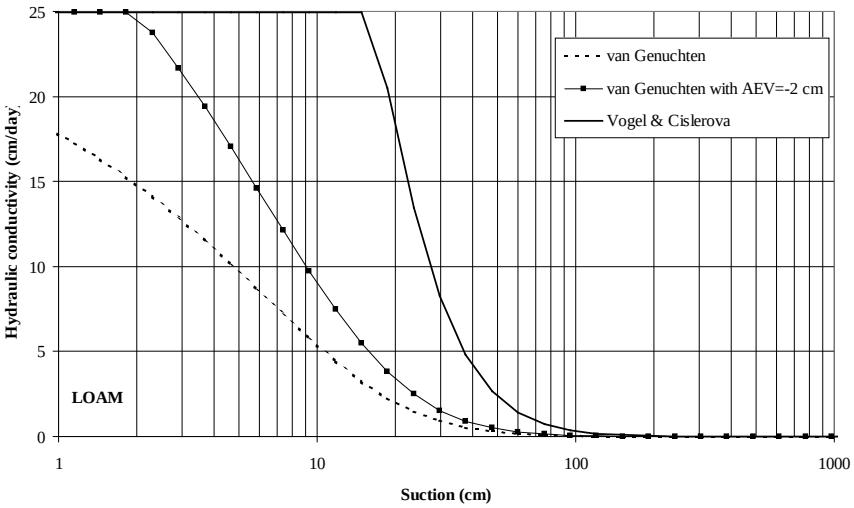

Figure III.8. The effect of the non-zero AEV on the hydraulic conductivity function.

Modified van Genuchten Model (Vogel and Cislerova)

When using this model, the hydraulic conductivity function is further discretized into three zones as shown in Figure III.9:

$h >= h_s$ (AEV)	$K(h) = K_s$
$h_k < h < h_s$	$K(h)$ is linear value between K_s and K_k
$h <= h_k$	$K(h)$ is non-linear (Mualem model)

where h_k is the head corresponding to a user-defined water content θ_k (Q_k in the HYDRUS GUI), θ_k is the water content below saturation where a measurement of the hydraulic conductivity K_k is available. The mathematical formulation for this model is found in the online Help and will not be repeated here. A comparison between the results of this model and the original van Genuchten model is shown in Figure III.10. Figure III.8 shows the significant differences near saturation. The modification was made to enable relatively large increases in K near saturation that are often observed in structured (macroporous) soils.

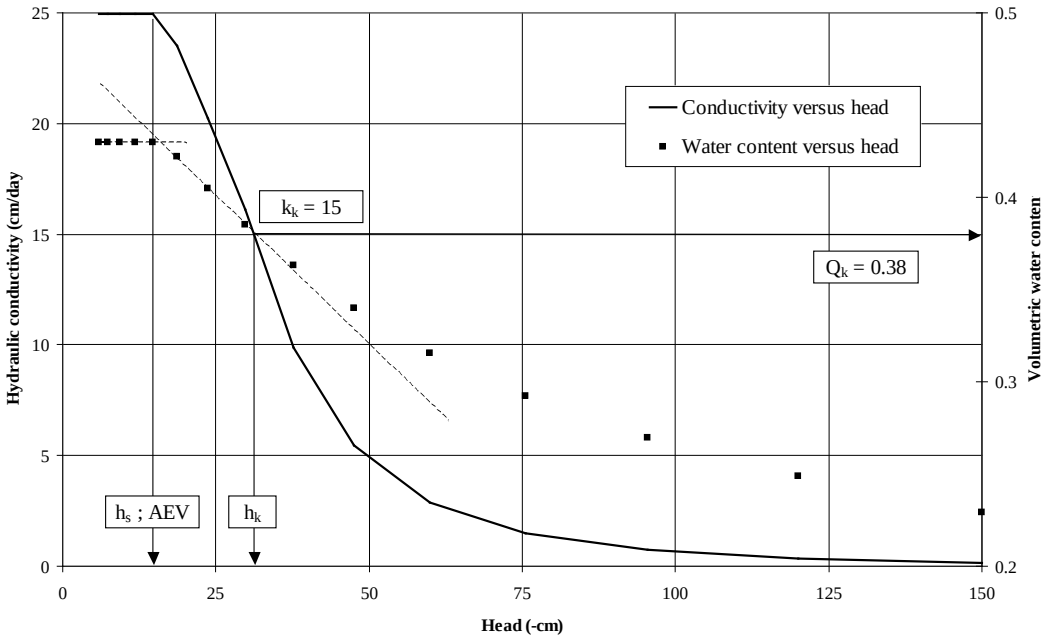

Figure III.9. The Vogel and Cislerova hydraulic conductivity function.

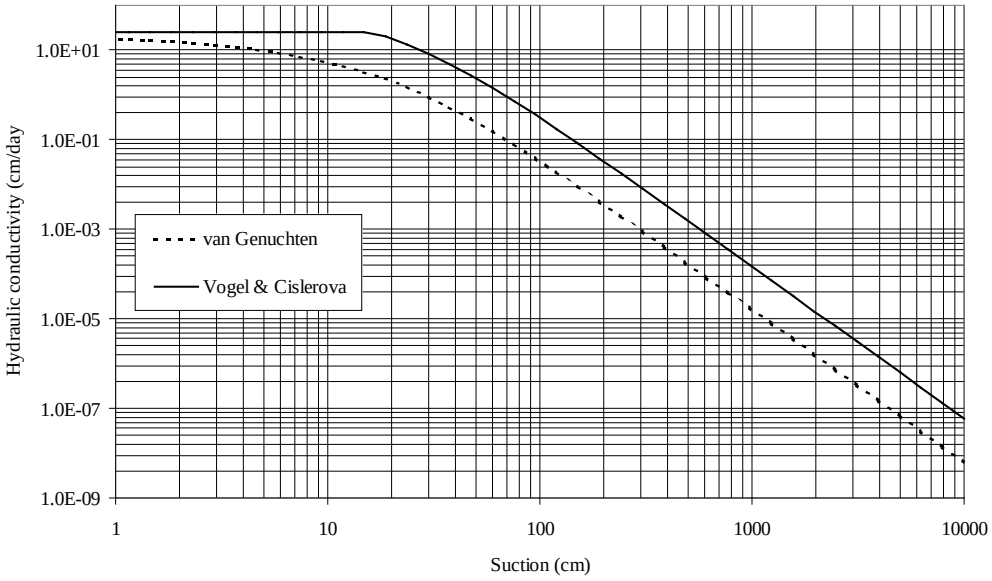

Figure III.10. The van Genuchten and Vogel and Cislerova hydraulic conductivity functions.

Brooks and Corey Model

For heads <AEV, the hydraulic conductivity is defined as follows:

$$K(h) = K_s \left(\frac{AEV}{h}\right)^{2+3n} \qquad \text{(III.7)}$$

A comparison of the results obtained with this model and those obtained with the van Genuchten model is shown in Figure III.11. The hydraulic parameters listed in Table III.1 were used for this purpose.

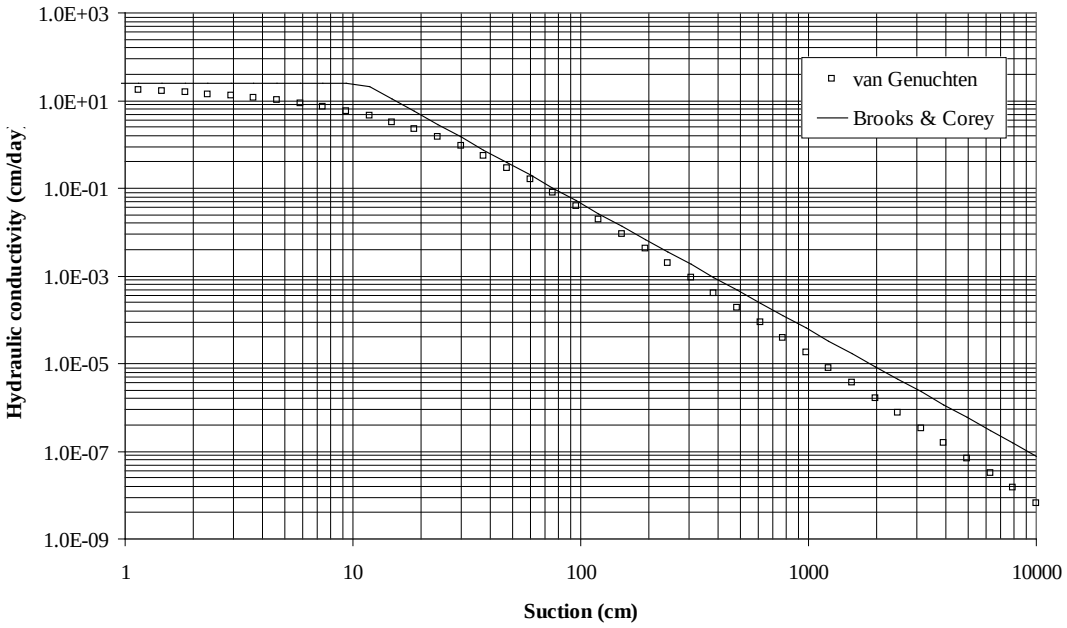

Figure III.11. The van Genuchten and Brooks and Corey hydraulic conductivity functions.

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CONTACT US

t 1300 363 400
+61 3 9545 2176
e csiroenquiries@csiro.au
w www.csiro.au

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FOR FURTHER INFORMATION

David Rassam
CSIRO Land and Water
Dutton Park, Brisbane
t +61 7 3833 5586
e david.rassam@csiro.au

Dirk Mallants
CSIRO Land and Water
Waite Campus, Adelaide
t +61 8 8303 8595
e dirk.mallants@csiro.au