HYPROP
Data Evaluation Software

User's Manual

DISCLAIMER

This manual documents the use of the HYPROP Data Evaluation Software, a computer program for analyzing data from evaporation experiments and fitting the unsaturated soil hydraulic properties. HYPROP Data Evaluation Software is a public domain code and may be used and copied freely. The code has been tested against a large number of soil hydraulic data sets, and was found to work correctly. 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

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1. Overview and Scientific Background

HYPROP – Data Evaluation Software (HYPROP-DES) is a software tool for Windows™ environment. The purpose of the software is to evaluate measurements obtained with the Evaporation Method by the UMS product HYPROP™. The software reads data that are recorded in TensioView projects by the data acquisition software "TensioView™ and stored in <.tvp> files. The files are converted to HYPROP-DES files with the extension <.bhd> (single measurement campaigns) or <.bhdi> (multiple measurement campaigns). HYPROP-DES performs the following operations:

(i)   Specification of all required parameters for the evaluation of the recorded experimental data, such as general information about project, column length, positions of tensiometers, weights of the measurement device and the used steel rings, and so on.

(ii)   Reading and visualization of the raw data, i.e., tensions and weight changes. The visualization includes the temporal interpolation of the discretely measured data.

(iii)   Calculation and visualization of the data for the retention characteristic and the conductivity characteristic.

(iv)   Fitting of hydraulic functions to the data, visualization of the functions, and listing of the confidence limits of the optimized hydraulic parameters .

(v)   Export of graphs, raw data, calculated data, fitted functions, and other parameters of interest.

The evaluation of measurement campaigns follows the simplified evaporation method. This method is used to determine hydraulic properties of soil samples in the laboratory, by evaluating the weight changes of samples and the matric potential in the samples during a drying process caused by evaporation. The principles of the method were first formulated by Wind (1968). A simplification of the Wind method, which is implemented in the HYPROP measurements, was proposed by Schindler (1980). Further advancements of the method are included in HYPROP-DES, such as the extension of the measurement range towards higher suctions by using tensiometers with boiling retardation (Schindler et al., 2010a), and a further extension of the measurement range by considering the air-entry value of the porous cups of the tensiometers (Schindler et al., 2010b). The validity of the simplified evaporation method has been investigated by Peters and Durner (2008). The detailed implementation of the method in the HYPROP-DES software follows the description given in that paper. It includes features that lead to an optimization of the method, such as a corrected fit of the hydraulic functions by the "integral method" to avoid bias in hydraulic properties near saturation (Peters and Durner, 2006), an Hermitian spline interpolation to the raw measured data to obtain smooth and continuous time courses of measured data, and an automatic detection the validity range of conductivity data in the range near saturation, where the hydraulic gradient becomes too small to yield reliable data. The simplified evaporation method yields correct results for soils where the water flow is validly described by the Richards equation with time-invariant hydraulic properties, and where hydraulic properties that can be described with the van Genuchten Mualem model (van Genuchten, 1980). For further information about the scientific background of the method, the reader is referred to the scientific publications listed in the references section. HYPROP-DES is freely available through the UMS website.

2. Installation of the Software

2.1 Installation using the Microsoft Installer

The easiest way to install the software would be to call up the file "HYPROP.msi" directly with the Explorer. Double-click on "HYPROP.msi". Then, follow the instructions on the screen of the installation assistance.

If you cannot execute the file "HYPROP.msi" you might need a current version of the Windows Installer® or/and .NET Framework 3.5 by Microsoft.

2.2 Access rights: Public User and Power User

HYPROP-DES is run in two user modes, which differ in the right to write or change parameters. "Public Users" run the software in a standard manner and apply default values for most specifications. "Power Users" are experienced and skilled users, trained in soil physics, and familiar with the scientific background of the data processing. A change of the user mode is done by selecting the appropriate mode at the lower right corner of the screen in a drop-down menu. A change of the user's status can be done at any time and from any register. It will immediately be active.

"Power Users" are allowed to alter many of the default values, or to manipulate measurement data. As an example, power users can edit or delete measured data records that are obvious outliers, or delete undesired records at the beginning or end of a measurement campaign. Furthermore, power users can process data that are measured on different devices, e.g. for evaporation experiments with different soil column heights. Changed parameters will affect the results of the data processing, and the implications on the calculations must be known by the users. In other words: if a Power User decides to alter parameters, he or she should really know what they are doing!

2.3 Language Selection

The HYPROP-DES GUI is available in English and German. A change of the language of the GUI is achieved by selecting the desired language in a drop-down menu at the lower right corner of the screen. A change can be selected from any of the registers, but to activate it, a re-start of the software is required.

3. Starting the Software and Loading a Project

3.1 Starting the program

To start the software, double-click the respective icon, or launch the software from the menu of installed programs. Upon the first start, an empty welcome screen will appear.
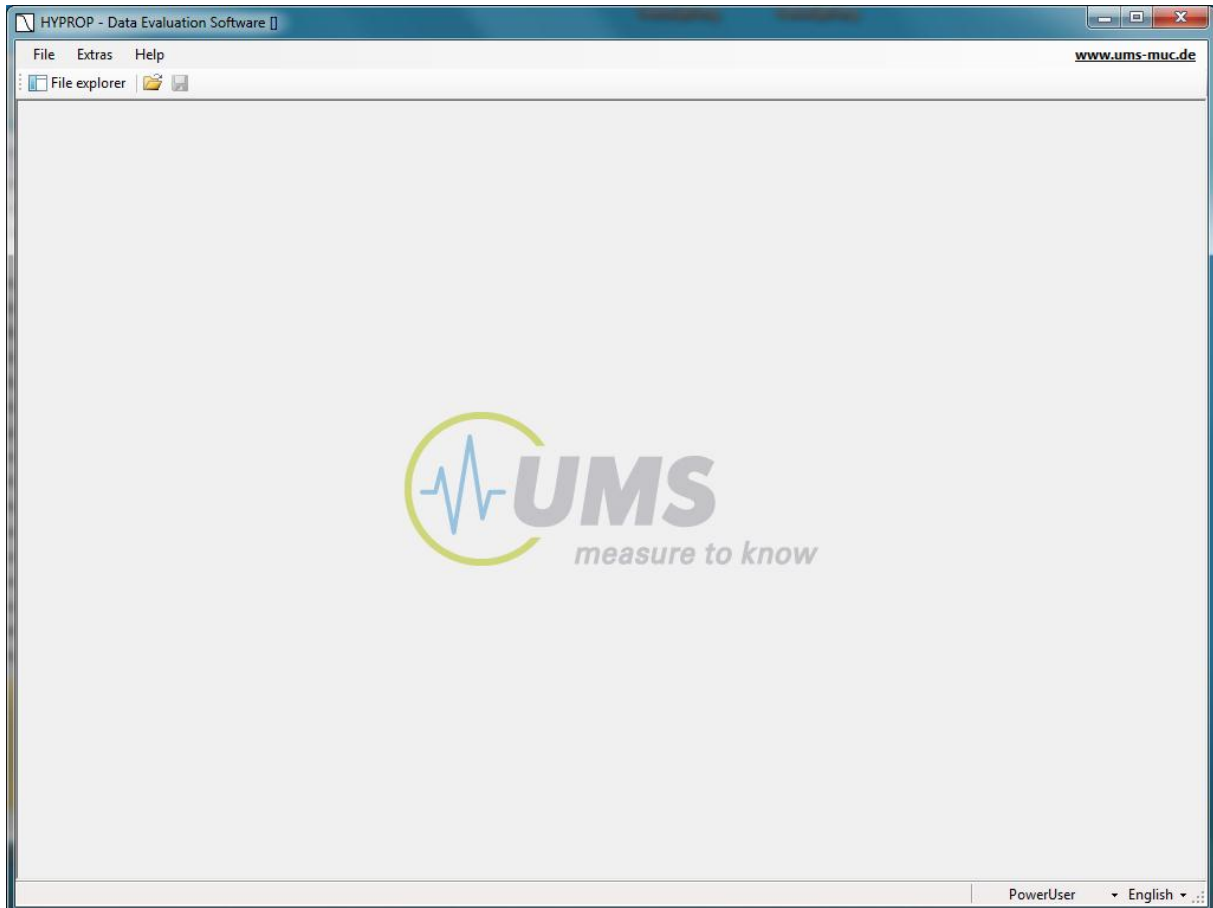
If previous data sets have been loaded, HYPROP-DSE will automatically load the last-used data set. If the last exit of the program was not regular (e.g., a crash caused by a corrupted data file), the program will again appear with an empty screen. The welcome screen shows three header lines:

(1) A top header line embedded in the blue window frame, which indicates the program name, with the project name in brackets (left), and the maximize, minimize and exit button (flushed right).

(2) A command line which contains three commands "File", "Extras", "Help" (left) and a link to the UMS website (right).

(3) An icon line with icons to open the "File explorer", and a "Open file" and "Save file" button.

Additionally the User level and the language of the software are depicted PowerUser   ▾ English ▾ to the right of the bottom line. The settings can be altered by selecting the respective option in the draw-down menus that open when clicking on the vertical triangles.

3.2 Opening, processing and storing projects - the commands File, Extras, Help
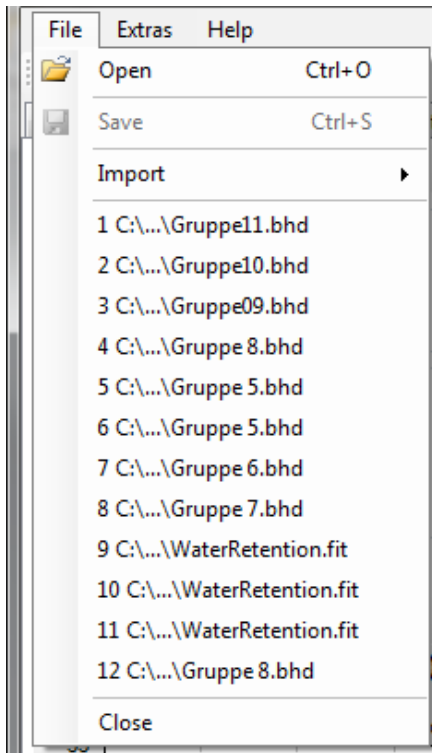
All command uses follow the standard Windows System conventions, as known from typical Windows GUIs. To perform the actions, position the cursor on a command or entry. The selected entry will be highlighted. It is launched by a single click with the left mouse key. Some commands are on-off buttons. An example is the "File explorer" button in the third header line. Clicking on it will lead to the pop-up of a file explorer window on the left of the main window, clicking on it again will lead to its disappearance. Other commands open submenus, where further commands or options can be selected. Commands that cannot be actively selected in a certain situation are shown in grey and cannot be used. As an example, the "Store file" button can only be used if a project has been opened and modified. Draw-down menus for selecting pre-defined options are indicated by vertical triangles on the right side of the respective button. Entries can sometimes be selected by key-combinations. If so, the combinations are indicated to the right of the respective entry. Menus can be left without any action by pressing the Escape button.

Three types of data can be processed:

- Raw data from TensioView measurement campaigns (.tvp) performed with the HYPROP experimental setup
- Existing projects of type HYPROP binary project (*.bhd), HYPROP binary iteration project (*.bhdi), or ASCII files (*_config.csv) with a predefined data structure.
- Separately measured retention and conductivity data in ASCII files (_RETC.csv and _COND.csv), or in a project file format (.fit)

3.2.1 Reading tensioVIEW project data from HYPROP measurement campaigns
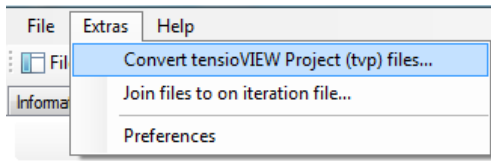
To import raw data from HYPROP measurement campaigns, open the submenu "Extras" and select the option "Convert tensioVIEW Project (tvp) files…". The imported raw data will be automatically converted to HYPROP binary projects of type *.bhd.
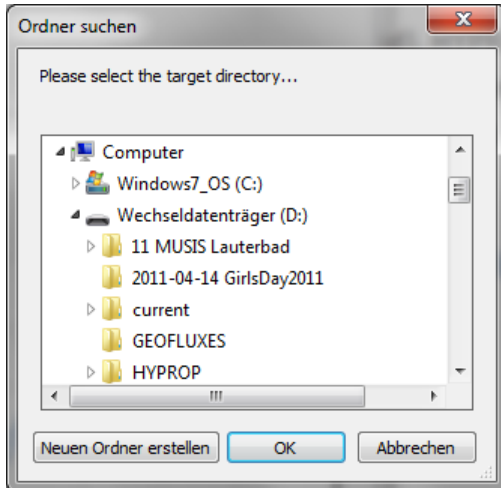
After the successful import, immediately the selection of a target directory for the storage of the *.bhd projects will be asked for.
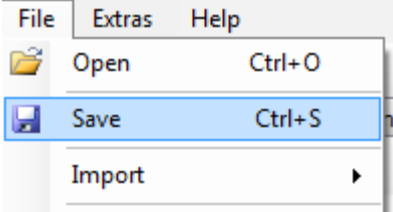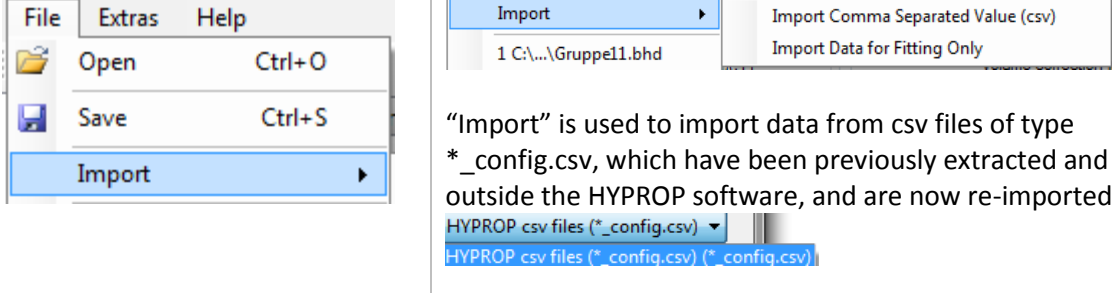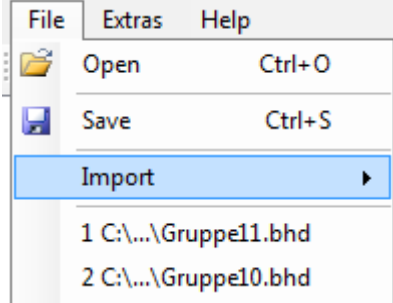
A new directory can be created and specified by pressing the respective button.

Depending on the measurement mode (single mode, multiple mode), one or more *.bhd files with the names of the measurement campaigns will be created in the target directory.

3.2.2 Menu "File" - Opening, modifying, and storing HYPROP projects

The menu "File" is used to open and save project files, and to import measurement of retention and conductivity data. An existing data file is loaded by selecting the respective file name in the open window, as described below. After opening a file, a fourth line with five registers will appear. The registers are entitled »Information«, »Measurements«, »Evaluation«, »Fitting«, and »Export«.

"Open" is the uppermost entry in the menu "File". Four types of data files can be opened:

HYPROP binary project files (*.bhd)
HYPROP binary iteration project files (*.bhdi)
csv files (*_config.csv) (*_config.csv)
All files (*.*)

.bhd   A HYPROP-DES binary project file, containing information, measurement data, calculated conductivity and retention data, and fitted functions for a single measurement campaign (DEFAULT)

.bhdi   A HYPROP-DES iteration project file, including data and fitted functions for multiple measurement campaigns.

.csv   csv files that contain HYPROP-DES dta in a structured manner. These files can be created in the "Export" register of the software (see section 5), externally modified, and re-imported.

All files (*.*) Shows files with any extension.

Only files with the selected extension will be shown in a browser window and can be opened by double-clicking on the

	name.
	"Save" is used to save a file which has been imported or processed. All changes will be saved. If no changes to an existing project have been made, the save button is inactive (grey shaded).
	"Import" is used to import data from csv files of type *_config.csv, which have been previously extracted and edited outside the HYPROP software, and are now re-imported.
	The subsequent group of entries in the File menu shows recently opened projects, allowing a direct and quick access to the projects by double clicking on the project name.
	"Close" closes the data file. If changes have been made, a confirmation to save changes is asked for.
Extras	This field currently contains no information. It is an empty field for future additions of extra commands.
Info	This field calls a screen that informs about the HYPROP-DES software, its version, and te developer team.

3.2.3 Menu "Extras" – Converting and joining files
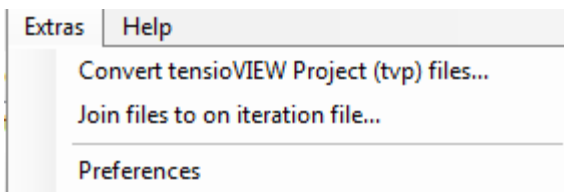
This menu is used to open tensioVIEW projects from HYPROP measurement campaigns, and to combine individual measurements to combined projects. Furthermore, it allows to pre-select preferences for the language and user type, and for the export of data.
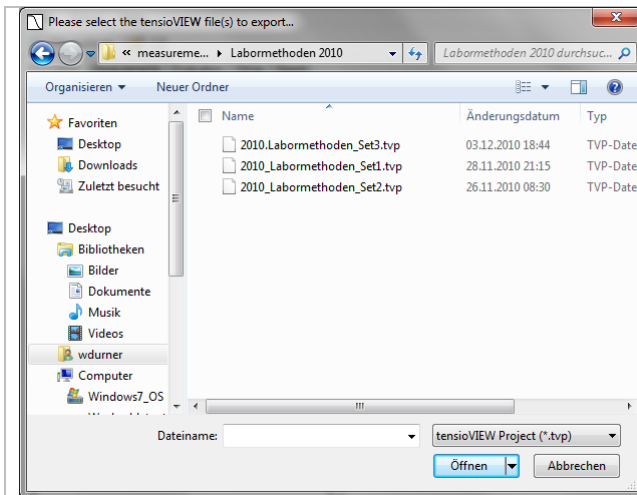
"Convert tensioView Project (tvp) files…" is used to read existing tensioView data files that have been produced by a HYPROP measuring campaign and stored by the data acquisition system in a tensioView project file.

It opens a browser window, from where the files that are to be imported can be selected.

The imported file will be immediately converted to one or more HYPROP binary data (bhd) files and can be stored and further processed.
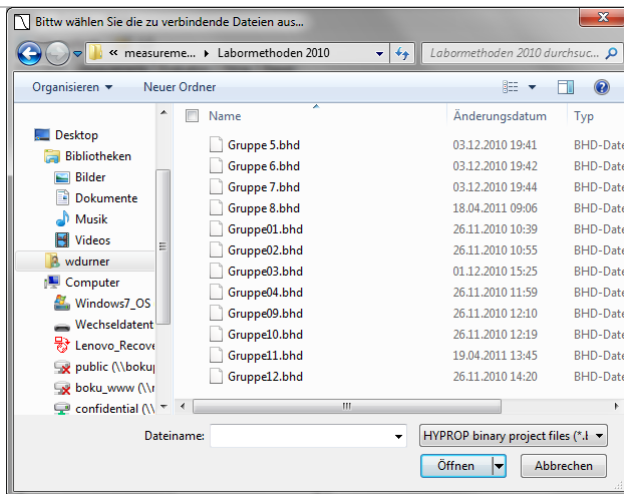
"Join files to an iteration file" is used to combine measuring campaigns that are stored as *.bhd files to one combined project file of type '.bhdi.

It opens a browser window, from where the files that are to be combined can be selected.

This is useful to compare different measurements and to fit retention and conductivity functions to multiple sets of data. Individual data sets will be shown in different colors, and can be switched on and off.
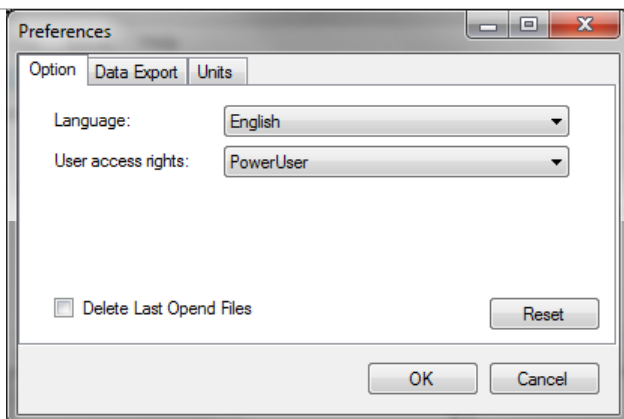
The "Preferences" menu contains three registers.

The first register "Option" is used to specify the default values for language and user mode: Power User (limited rights for manipulating HYPROP_DES parameters, referring to generally valid default values) or Public User.

The second register "Data Export" specifies a variety of conventions for the export of data, such as regional and language options and data separators.

The third register "Units" is currently empty and will be used in a later version of HYPROP-DES to specify the preferred units for pressure head, conductivity, and water content.

3.2.4 Menu "Help" – HYPROP-DES version information

The submenu "Info" in Help shows the used version of the HYPROP Data Evaluation Software, lists the HYPROP development team, and shows the disclaimer.
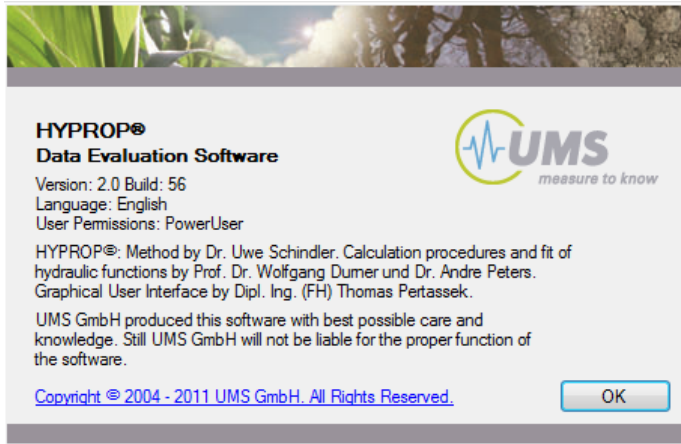
4. The Registers – Processing Data

The HYPROP-DES software groups the data processing in five registers that encompass all steps of the data evaluation in a logical sequence of consecutive operations. Normally, the registers are followed consecutively from left to right. In all registers, data processing options can be specified, and data can be edited or manipulated.

Common to all registers are the following points:

- Editable values are shown in a edit field, i.e., surrounded by a frame with a slightly brighter background
- Values that cannot be modified are just shown without the edit field.
- All variables that are expressed by numerical values are given with units. If a value is edited by the user, the inserted numerical value must be in the given unit
- Whether or not a variable can be edited depends on the user mode: power users can edit more fields than public users.
- When inserting a numerical value, the proper decimal separator sign depends on the region settings of the computer. Default for the Germany version is the comma, whereas default for the English version is a dot.
- Fields for numerical values do not accept input of alphabetical letters or special signs; if a user attempts to insert a non-permitted character, the field does not show the typed character.
- To be sure that an input operation is finished, the cursor must have left the leave the input field. This is achieved either by pressing the Tab-Key, or the Return key, or by moving the curser to another position in the window and clicking the left mouse button. In some menus explicit pressing of an "Accept" button is required.
- When placing the cursor on a button, a specific text information (Quickinfo) about the button's function pops up for a period of some seconds.
- Some of the graphs and other contents have context-sensitive menus that are activated by placing the cursor on them and a right-click of the mouse.

4.1 Register »Information« – Specifying the required parameters for the measurement

The »Information« Window contains nine groups of information blocks about the project. Some of the data are editable by the "Public User", some more are editable by the "Power User", and others that cannot be altered by the user and are listed as information that is specified by the TensioView data acquisition program and the respective firmware.

In a typical measurement evaluation, there is one single input value that must be specified by the user in this window: This is in group five "HYPROP Parameter" the Soil sampling ring weight [g]. Since the sampling ring weight differs from sample to sample, the weight of the ring must be specified for each individual measurement. As default value, the average weight (201 g) is given, but differences of the actual weight to this default value will affect the initial water content calculation.

In the following, the data groups will be listed and the inputs will be explained.

Data group General Information

Variable	Explanation	default value	editable by public user	editable by power user
Sample Name	Denomination of a sample. The name can be chosen freely by the user. It should be noted, that the sample name is used for the creation of the filename during export by default. The filename rules have to be considered. If data stem from a HYPROP measurement campaign with tensioVIEW, the sample name specified in tensioVIEW is listed here.	From HYPROP campaign	Yes	Yes
Start of measurement	Date and time from the start of the recorded data. These data are given by the .tvp file.	-	No	No
Stop of measurement	Date and time from the end of the recorded data. These data are given by the .tvp file.	-	No	No
Duration of measurements	Difference between end and start date of the recorded data, calculated from the two fields above and rounded to full days		No	No

Data group Correction

Variable	Explanation	default value	editable by public user	editable by power user
Volume Correction	Correction of the sample volume. This can be necessary e.g., if the prepared sample surface is not perfectly prepared and shows deficits (negative correction), or if swelling occurred during saturation and the user decides not to cut the saturated sample to exactly 5.0 cm height. Volume correction will affect the calculation of the water contents, since the weight changes will be related to the value "Volume"+"Volume correction".	0 cm³	No	Yes
Weight correction	Addition (positive) or subtraction (negative) of a constant weight to the Tare weights, i.e., to the measuring head and the sample ring weight, which are subtracted from the total weight to obtain the net sample weight. This could be the constant weight of, e.g., a lid, a cable, or another sensor that might be added in a measurement campaign. This Variable is of particular importance in HYPROP measurement campaigns that were performed in the **"Single Mode".** Note that in these cases the weight of the cable connection (often around 7 g) must be inserted in this field	0 g	Yes	Yes

Data group Zero Offset correction

An offset correction is required, if the user has a clear indication that the calibration of a tensiometer is not correct. In general, the tensiometers must show under hydrostatic conditions with the water level equal to the upper end of the sample tensions (= negative of the matric potential!) of -1.25 hPa (upper) and -3.75 hPa (lower position). The difference of the two tensiometers thus will be 2.5 hPa in

the initial measurement phase. Deviations from this difference will strongly affect the calculation of the conductivity values. If values under these experimental conditions are different, it is possible to correct the whole data set for a constant shift. The correction will be added to all recorded tensions.

WARNING: Be careful! Please correct tensions to assumed hydrostatic conditions only if you are certain that these conditions were actually prevailing at a given time of your measurement campaign.

Upper tensiometer	Added offset for the measured values of the upper tensiometer.	0 hPa	No	Yes
Lower tensiometer	Added offset for the measured values of the lower tensiometer.	0 hPa	No	Yes

Data group Geometric Parameters

Geometric Parameter
Soil volume [cm3]: 249
Soil column height [cm]: 5,00
Position lower tensiometer [cm]: 1,25
Position upper tensiometer [cm]: 3,75

HYPROP Parameter
Soil sampling ring weight [g]: 201,0
Measure head net weight [g]: 358,0
Air entry pressure upper tensiometer [bar]: 8,8
Air entry pressure lower tensiometer [bar]: 8,8
Density of solid substance [g/cm3]: 2,65

Measurement Uncertainty
Tensiometer [hPa]: 0,60
Scale [g]: 0,06

Variable	Explanation	default value	Ed. by public user	ed.by power user
Soil volume	Volume of soil sample. Default value is given by UMS standard sample rings (250 cm³) minus the volume of the two tensiometers (1 cm³)	249 cm³	No	Yes
Soil column height	Height of soil sample. Default value is given by UMS standard sample rings.	5 cm	No	Yes
Position lower tensiometer	Position of the lower tensiometer in the sample, measured from the base of the sample. Default value is valid for the UMS HYPROP device, where the lower tensiometer is located at ¼ of the total height.	1.25 cm	No	Yes
Position lower tensiometer	Position of the upper tensiometer in the sample, measured from the base of the soil sample. Default value for the UMS HYPROP device is ¾ of the sample height	3.75 cm	No	Yes

Data group HYPROP Parameters

Soil sampling ring weight	Exact mass of the soil sampling ring (dry and clean). IMPORTANT: THIS VALUE MUST BE SPECIFIED INDIVIDUALLY FOR EACH MEASUREMENT CAMPAIGN! The mass can be determined before or after the HYPROP measurement campaign. The default value is the mean value of the first series of sample rings provided by UMS. Wrong values transfer linearly to wrong calculated total water contents. An error of 2.5 g leads to a shift of calculated water contents of 1%.	201 g	Yes	Yes
Measurement head net weight	Mass of the dry, clean measurement base. The mass includes the two filled tensiometers and the silicon sheet that is used to separate the head from the	258 g and 261 g	No	Yes

	measurement base, but with no water below the sheet. Normally, the weight is accurately derived from the default that is dependent on the serial number of the head. If uncertain, then perform a control measurement. Wrong values transfer linearly to wrong calculated total water contents. An error of 2.5 g leads to a shift of calculated water contents of 1%.			
Air entry pressure upper tensiometer	This value specifies the air entry pressure of the cup of the upper tensiometer. The value is used if the "use air-entry" option is activated (power users only). The default value is the statistical mean of ceramic cups used in the 2010 series of UMS HYPROP tensiometers. For individual specifications, please follow the detailed instructions given by Schindler et al. (2010).	8.8 bar	No	Yes
Air entry pressure lower tensiometer	As above, for tensiometer at lower position.	8.8 bar	No	Yes
Density of solid substance	The density of the solid soil material is by default set to the density of quartz, i.e., 2.65 g/cm³, which in general is a good approximation for a wide range of soil materials. If individual measurements for the soil under investigations are available, this value can be replaced by a measured one. The value is used to calculate the porosity of the sample from the dry soil weight. It is also used for the "automatic" estimation of the saturated water content, as described in Appendix 2.	2.65 g/cm³	No	Yes

Data group Measurement Uncertainty Parameters

Variable	Explanation	default value	editable by public user	editable by power user
Tensiometer	Statistical measurement uncertainty of the tensiometer, i.e., standard deviation of repeated tensiometer readings at a constant physical pressure head. The tensiometer reading uncertainty is used to calculate the parameter uncertainty of the results, as indicated by the confidence limits given in register "fitting".	0.6 hPa	No	Yes
Scale	As for the tensiometer. The uncertainty of the scale readings transposes to uncertainties of the calculated water contents, and thus affects the uncertainty estimates for the optimized functions parameters in register "fitting".	0.06 g	No	Yes

Data group Sensor Unit Information and Scale Information

Note: the information in these parameter groups is not affecting the calculations; values are given purely for information purposes.

Variable	Explanation	default value	editable by public user	editable by power user
Serial number	Information given by UMS firmware through .tvp file	-	No	No
Sensor unit name	Information as specified in data acquisition and stored in the .tvp file	-	No	No
Busnumber	Information as given in the data acquisition and stored in the . tcp project file. Busnumber can be modified in the TensioView data acquisition software. This can be necessary in the ulti-head mode, for the seldom case that default bus numbers of two measuring heads are equal.	-	No	No
Subaddress	Information given by UMS firmware. As above.	-	No	No
Tensiometer Version	Information given by UMS firmware	-	No	No
Firmware Version	Information given by UMS firmware	-	No	No

Data group Scale Information

Note: the information is not affecting the calculations; values are given purely for information purposes.

Serial number	Information given by UMS firmware through .tvp file	-	No	No
Scale name	Information as specified in data acquisition and stored in the .tvp file	-	No	No

Data group Notes

Description	Any information in tabular view	-	Yes	Yes
Value	Any information in tabular view	-	Yes	Yes
Free data field	Here, any informative text can be stored that is usefully related to the measurement campaign.	-	Yes	Yes

4.2 Register »Measurements« - Visualization and editing of measured data
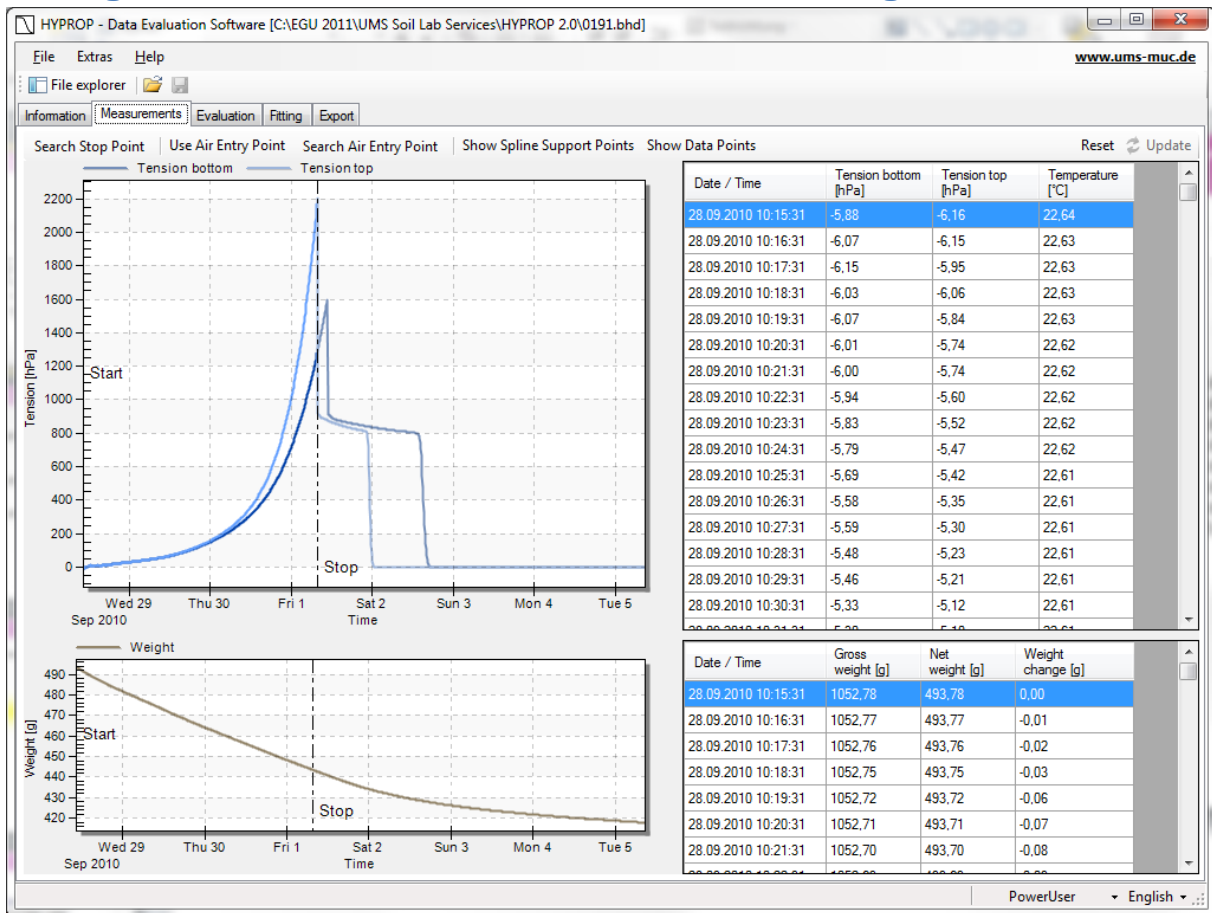
The register "Measurements" shows the readings of the two tensiometers and the recorded weights. The register is composed of four windows. Two of the windows show graphs of the recorded data, two others the numeric values. The size of the windows can be freely scaled by positioning the mouse on the (invisible) borders of an individual window and dragging the border to a new position. If the mouse is directly on a border, its appearance changes from the arrow to a double arrow. Each of the graphics windows can be enlarged to full-screen by positioning the mouse on the window, clicking the right-hand mouse button, and selecting the respective option in the pop-up menu. Leaving the full-screen mode is reached by pressing the Escape key. A user can (repeatedly) magnify portions of the graphs (regardless whether in windows of full-screen mode) by placing the mouse on the graph, and drawing the cursor to the opposite point of a rectangle with the left mouse button held down. To reset the window ranges, click the right-hand button of the mouse and select the respective option.

4.2.1 Interpretation of the tensiometric data

In a long measurement period, as shown in the example screen, we see after an initial reaction and a plateau phase an exponential increase of both tensions, steeper for the upper tensiometer, which is followed by a sudden collapse to smaller values. This collapse occurs upon cavitation of the water phase in the tensiometer, which causes the pressure inside the tensiometer to suddenly jump to the vapor pressure of water. Before this cavitation, the water in the tensiometer is due to boiling retardation under a strain, i.e., under negative absolute pressure. To measure this sharp cavitation point at tensions > 1000 hPa, tensiometers must be well prepared, without any gas bubbles inside, as

indicated in the HYPROP manual. The recorded values are absolutely reliable up to the cavitation point. Accordingly, the cavitation point of the upper tensiometer marks the end of the data that can be directly evaluated. This "stop point" is automatically detected by the software and indicated by a vertical dashed line. The stop line can be manually shifted to an earlier or later time be placing the mouse cursor on the stop line, and dragging it to the left or to the right. The automatic detection of the stop point can again be applied by clicking on the "Search Stop Point" button immediately above the graph.

If tensiometers were not well prepared, the boiling retardation is not reached and the sudden collapse is not visible, but replaced by an asymptotic approach of the tension towards a final value. In these cases, the automatic stop point detection is not fully reliable, and users must carefully check the end position. As a rule of thumb, and end point at approx. 80% of the maximum tension is recommended.

After a certain time with further evaporation, the tensiometer cups will dry out and become permeable to air. At that time, the absolute pressure inside the tensiometers will increase from the vapor pressure to the pressure of the ambient atmosphere. Accordingly, the recorded tension will collapse to zero.

4.2.2 Data Visualization Options

| Information | Measurements | Evaluation | Fitting | Export |

| Search Stop Point | Use Air Entry Point | Search Air Entry Point | Show Spline Support Points | Show Data Points | Reset ⟳ Update |
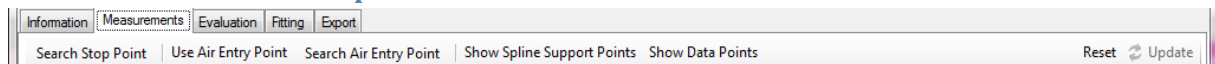
In the header line above the graphs, buttons for data visualization options are listed. They differ for power users and public users. The options are as follows:

Search Stop Point	The stop point of the measurement is reached by the cavitation of the upper tensiometer, which is indicated by a sudden pressure drop. HYPROP-DES detects this point automatically. If the Stop-line is moved manually to another time, it will be reset to the automatic detection by pressing the "Search Stop Point" button again. If the tensiometer is not filled correctly, the drop might not occur in that sharp manner, since the tensiometer does not reach a tension. In that case it might be necessary that a user chooses the Stop point manually. A good choice is then to select the point with the highest slope of the upper tension.	Automatic	No	Yes
Use Air Entry Point	Activates and deactivates the use of the air-entry point of the porous cup as additional tension value, as described in section 4.2.4.	No	No	Yes
Search Air Entry Point	If the "User Air-Entry Point" is activated, and the line that indicates the time of the air-entry point has been moved manually, pressing this button resets the automatic detection of the air entry time.	-		

Show Spline Support Points	Activates and de-activates the depiction the supporting data points, as described in section 4.2.3	-		
Show Data Points	Activates and de-activates the depiction of the individual measured data points, as described in section 4.2.3	No	Yes	Yes
Reset	The option "Reset" resets all settings to default values, in particular the ranges for the visualization of the data in the two graphs.	-	Yes	Yes

4.2.3 The tension graph

The upper graph is the tension graph that normally shows two lines. The bright blue line indicates the tensions recorded by the upper tensiometer versus time, the dark blue line the corresponding course of the lower tensiometer. The x- and y-axes are automatically scaled to show all recorded data.

Visualizing measured datapoints

The graph shows by default the temporal evolution of the tensions as lines, without individual dots for the data. If desired, a user can visualize additionally all individually recorded data by moving the cursor on a line, right-hand clicking the mouse, and selecting the respective option from the context-sensitive pop-up menu. De-selecting the option leads the individual data points again to disappear. Data can also be shown by clicking on the respective on-off button in the header line directly above the graph.

Visualizing the supporting points used for the smooth interpolation of the data

As indicated in Peters and Durer (2008), not all data are used for the calculation of the retention and conductivity data, but just a limited number of support data that defines a Hermitian spline interpolation. The actual number of these data can be selected by the user in the submenu "Interpolation Options" in the register "Evaluation" (see below). Supporting data can be visualized by clicking on the on-off button "Show Spline Support Points" in the header line directly above the graph.
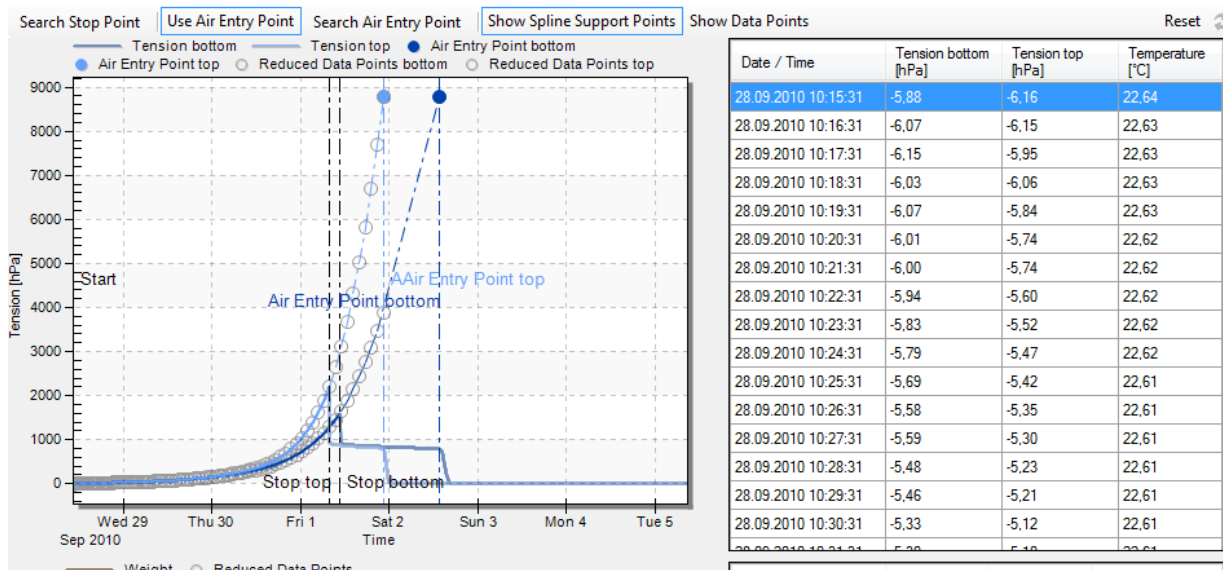
4.2.4 Using the air-entry point of the tensiometer cup as additional tension measurement (Power User only)

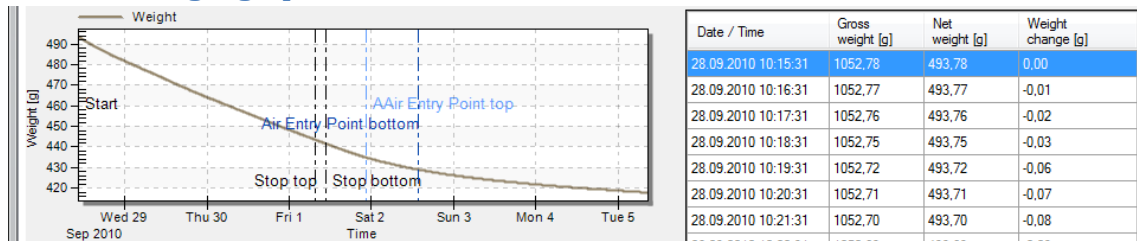It is possible to extend the range of the tensiometric measurements by using the air-entry value of the ceramic tensiometer cup as additional measuring point (Schindler et al., 2010b). The HYPROP-DES includes this option for Power Users. The air-entry point is located at the sudden pressure drop of the tensiometers towards zero (Fig. 1). Of course, this option is only viable if the sharp drop towards zero tension is really recorded, i.e., if the measurement campaign was performed long enough.

Clicking on the "Use Air Entry Point" button will add for each tensiometer (for which this) a new measuring point that is on the temporal axis located at the drop of the tension, and on the y-axis at a tension that was specified in the register "Information"- "HYPROP-Parameters". The button "Use Air Entry point" is an on-off switch. Hence, to deactivate the use of the air-entry point, press the button again. At the time of the air-entries of the two tensiometers, vertical lines will be shown. If the drop of the tension is not clearly indicated by the course of the data, the automatic detection of the air-entry point will fail. The vertical air-entry line is then at a wrong position, but can be moved with the cursor, as described above for the stop point position. After manual shifting, the original position due to the automatic detection can be again recovered by pressing "Search Air Entry Point".

When the "Use Air Entry Point" option is active, dashed lines are shown that interpolate the tensiometric data between the last reliably measured points (stop point) and the air entry points of both tensiometers. For the HYPROP-DES calculations, the tensiometric value of the lower tensiometer will be taken from this interpolation. For further information about using this option, the user is referred to the publication of Schindler et al. (2010b).

4.2.5 The weight graph

Date / Time	Gross weight [g]	Net weight [g]	Weight change [g]
28.09.2010 10:15:31	1052,78	493,78	0,00
28.09.2010 10:16:31	1052,77	493,77	-0,01
28.09.2010 10:17:31	1052,76	493,76	-0,02
28.09.2010 10:18:31	1052,75	493,75	-0,03
28.09.2010 10:19:31	1052,72	493,72	-0,06
28.09.2010 10:20:31	1052,71	493,71	-0,07
28.09.2010 10:21:31	1052,70	493,70	-0,08

The lower graph is the weight graph. It shows a grey line that indicates the net weight of the sample, i.e., the mass of dry soil plus the mass of water. The accuracy of the absolute level of these data depends on the accuracy of the values for the measurement head and the steel cylinder, and possibly additional weights, as described in the register "Information". The accuracy of the weight changes, i.e., the relative accuracy, is equal to the accuracy of the used scale. The times of the Stop and the Air-entries are shown by vertical lines, at identical positions to the tension graph.

The x- and y-axes are automatically scaled to show all recorded data. Parts of the graph can be manually enlarged and reset as described for the tension graph. Note that changing the time axis of the weight of one graph does not affect the tension graph, and vice versa.

Visualization of the actually measured points and the spline support points can be activated and de-activated as described for the tension graph.

Interpretation of the weight data

In a typical measurement, the weight data will first show a continuous weight loss with an almost constant rate, which reflects the evaporation rate in the laboratory environment. Small changes in the slope can be caused by temperature fluctuations in a lab, with the respective changes in relative humidity. The period of a constant weight loss rate is called "Phase 1" evaporation, and water loss during that phase is controlled by atmospheric conditions. Afterwards, the rate drops, and the slope of the weight curve becomes less steep. This second phase is called "Phase 2" evaporation. The water loss rate is now controlled by the resistance of the drying soil near the soil surface. In the depicted data example, the phase 3 evaporation starts at the time when the upper tensiometer reaches its air-entry value. For further information see Peters and Durner (2008), and Schindler et al. (2010, 2011).

4.2.6 The tension data window

The window at the upper right shows the recorded tensiometric data, together with the times and the temperature. The latter is for information purposes, and not used in the data evaluation. The data window can be scrolled by the scroll bar to the right. By moving the cursor into the data window, and clicking on the right-hand mouse button, the data can be directly edited by Power Users. Possible operations are deletion of lines, insertion of lines, and changes of the contents of individual data cells. Also, multiple lines can be selected, and the data can be copied with the "ctr+c" option. Manipulation of data or deletion of data will be immediately shown in the graph to the left.

4.2.7 The weight data window

The window at the lower right shows the recorded weight data. After date and time (column 1), the total weight of the measuring system, including all tare weights is listed (column 2). The net weight of soil plus water is calculated from the total weight minus the tare weights, as specified in the "Information" register, and listed in column 3. These data are also depicted on the graph to the left. Finally, the net weight change from the start of the experiment is listed in column 4. The data window can be scrolled by the scroll bar to the right. By moving the cursor into the data window, and clicking on the right-hand mouse button, the data can be directly edited by Power Users. Possible operations are deletion of lines, insertion of lines, and changes of the contents of individual data cells. Also, multiple lines can be selected, and the data can be copied with the "ctr+c" option. Manipulation of data or deletion of data will be immediately shown in the graph to the left.

4.3 Register "Evaluation" - Calculating retention and conductivity data
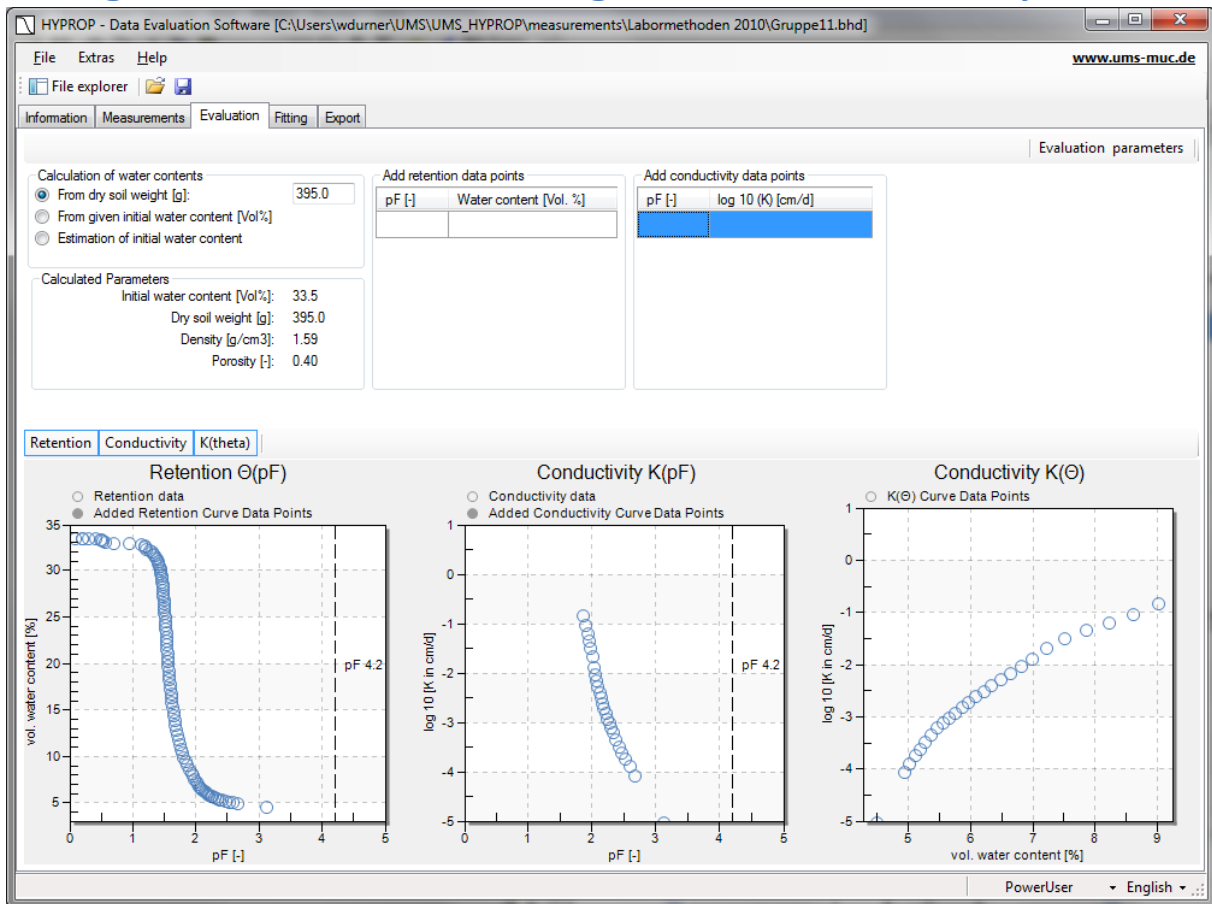
The register »Evaluation« shows in the upper part four data groups with specifications for the calculation of absolute water contents, calculated parameters, and two menus for adding additional data points. In the lower part, up to three graphs of the resulting retention and conductivity data are shown. The first graph shows the volumetric water content versus pF (== decimal log of tension, expressed as pressure head in the unit of cm). The second graph shows the log of the hydraulic conductivity versus pF, and the third graph the log of hydraulic conductivity versus volumetric water content. The individual graphs can be switched on or off by pressing the respective buttons that are located immediately above the graphs, to the left. Switching a graph on or off will resize the remaining graphs.

4.3.1 Calculation of retention and conductivity data

The calculation of retention and conductivity data from the measured tensions and weight changes follows the simplified evaporation method as outlined by Schindler (1980), Schindler et al., (2010a,b) and Peters and Durner (2008). For the theoretical background of the calculations, the reader is referred to this literature. In the calculations, only the tensions and weights in the time window between start time and stop time, which is specified in the previous register "Measurements", are considered.

4.3.2 Calculation of absolute water contents

The relative position of the water retention data is fully determined by the recorded weight change. The absolute level of the water retention data is additionally affected by the parameters that can be specified in the parameter group "Calculation of water contents".

Option1: Calculation of the initial water content from dry soil weight

This is the option of choice if the dry soil weight has been determined after the end of the measurement campaign, by oven-drying at 105°C for 24 hours. The exactness of the results depends on the correctness of all involved parameters that are specified in the "Informations" register. From the data, further soil physical parameters such as the initial water content, the identical porosity, the dry bulk density, and the dry soil weight are also calculated and shown in the underlying group "Calculated Parameters". Note: **Only option 1 leads to a correct calculation of the absolute water contents.**

Option 2: External setting of the inital water content by user

This option allows a user to externally set the initial water content to a desired value (from wherever he takes this value). Since the saturation state associated with the externally set initial water content is unknown, no calculation of porosity, dry bulk density and dry soil weight is possible, and no values of these parameters can be shown.

Option 3: Automatic estimation of the inital water content

If the dry weight of the soil is not yet available, the initial water content of the campaign can be estimated automatically by the software assuming an initially full saturation of the pore space (i.e., initial saturation = 100%). In practice, this will rarely be reached; the calculated water content is therefore to be seen as an approximation of the true one. Furthermore, the calculation depends on

the correctness of all involved parameters that are specified in the »Information« register, in particular on the correct dry bulk density (DEFAULT 2.65 g cm^{-3}), mass of the measuring head (DEFAULT 358 g), and mass of the steel cylinder that contains the sample (DEFAULT 201 g). Any error in these data will be linearly transferred to the results. As a result of the assumptions, the initial water content, the identical porosity, the dry bulk density, and the dry soil weight can be calculated. These values are shown in the underlying group "Calculated Parameters". Details of the automatic calculation are given in Appendix 2.

If the mode of the initial water content calculation is changed, the user-edited values for the dry soil weight and for initial water content remain in storage. This allows a user to switch between the options and to conveniently compare the outcomes of the different calculation options, without losing the inserted information.
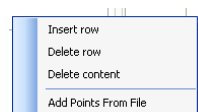
4.3.3 Adding independent retention and conductivity data

Users can add independently measured data, e.g., from WP4 measurements or from pressure plate measurements. This is done by typing the value in the respective field. To complete the insertion, the cursor must be positioned out of the field, which can be done by pressing the "Tab" or "Return" key or by moving the mouse to another field. The additional data are shown immediately in the data graphs by solid markers, whereas the HYPROP calculated data are shown as empty circles.

IMPORTANT! Please care for the appropriate units when adding the data: tensions must be added as pF, water contents in percent, and conductivity data as decimal log of the value expressed in cm per day. Also please care for the regional conventions for the decimal separator (comma or dot), as specified in the Windows System Software. Added data can be edited and deleted. Upon a right-hand mouse click, a pop-up menu appears:

As an additional feature, retention and/or conductivity points can be read from data files of type .csv. This is of particular advantage if many points are available from independent measurements.

4.3.4 Modifying evaluation parameters (Power User only)
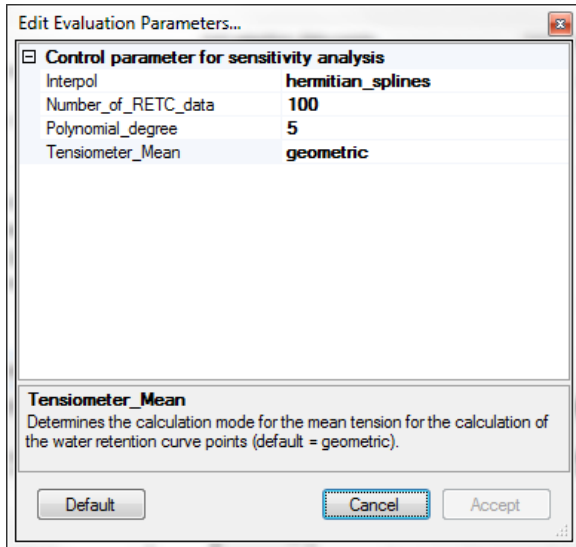
The parameters for raw data interpolation can be edited in a submenu Edit Evaluation Parameters... ,
which pops up when clicking on the respective button on the right side of the header line in register
»Evaluation«. The interpolation parameters are described below.

General Information

Variable	Explanation / possible values	default value	editable by public user	editable by power user
Interpol	Determines the interpolation mode for the measured data: 0: polynomial 1: piecewise linear **2: hermitian splines**	2	No	Yes
Number_of_ RETC_data	Number of support points for hydraulic functions (< 1000)	100	No	Yes
Polynomial degree	If Interpol is set to 0, then the degree of the polynomial used	5	No	Yes
Tensiometer_mean	Determines the calculation mode for the mean tension for the calculation of the water retention curve points: 1: arithmetic **2: geometric,** 3: harmonic.	2	No	Yes
Tpower	Determines the spacing of the support points for the spline interpolation. A vlaue of 1 means equal spacing in time, a value of 0.5 means a spacing that is proportional to the square root of time. Recommended values are between 0.5 and 1.	0.75	No	Yes

4.4 Register »Fitting« - Fitting hydraulic functions to the data
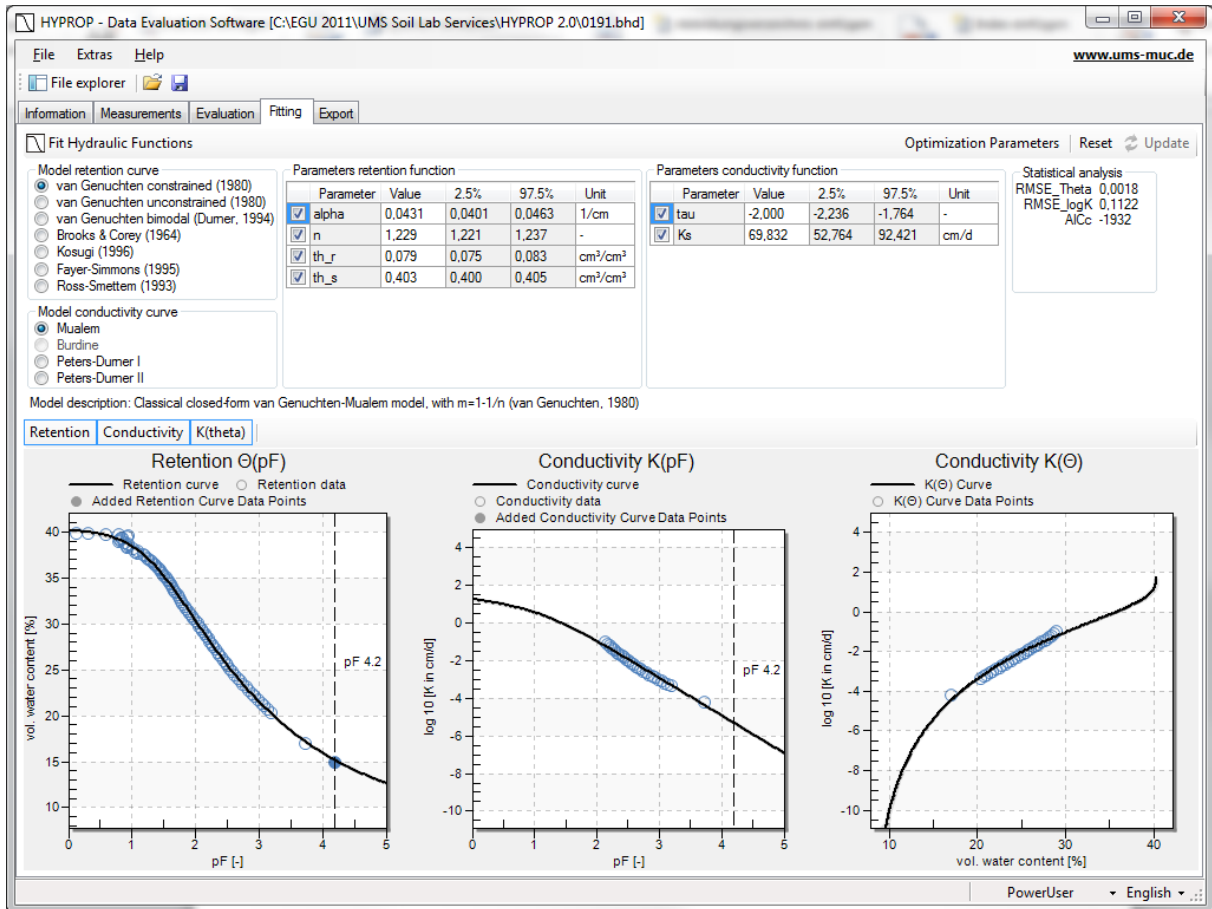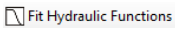
For use in numerical modelling, hydraulic characteristics are described by parametric functions for θ(h) and K(h), or K(θ). HYPROP-DES provides a high-class algorithm to fit functional relationships of the retention curve and the conductivity curve to the data. No specification of initial guesses for the parameter values is requried. Seven widely used retention models are available, encompassing expressions for soils with unimodal (van Genuchten, Kosugi) and bimodal (Durner, Ross-Smettem) pore-size distributions, with (Brooks-Corey) and without distinct air-entry, and a model extension that reaches water content zero at pF 7 (Fayer-Simmons). The retention functions are coupled to conductivity models by the classical pore-bundle models of Burdine (1953) and Mualem (1976), including a film-flow component according to the models of Peters and Durner (2008). All models are described in detail in appendix 3.

4.4.1 Fitting functions

The "Fitting" register contains a header line with the fit button at left ("Fit Hydraulic Functions"), and buttons for "Reset" and editing of "Optimization Parameters" to the right. The data to be fitted are shown together with the fitted functions in the graphs in the lower part of the window. The non-linear parameter optimization is subject to constraints and settings, which are defined in the

submenu "Optimization Parameters" (see 4.4.3). The "Reset" button will reset all values for the parameter bounds to the default values.

To fit the selected hydraulic functions (see 4.4.2) to the data, click on the ⬚ Fit Hydraulic Functions button. A window will pop up that indicates that the fitting routine is running. This process can take seconds (for the simple models with few parameters) up to minutes (for complex models with many parameters), and cannot be stopped or otherwise interrupted[1].

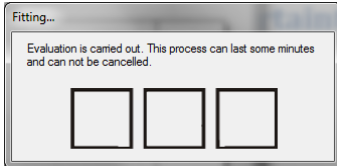The fitting algorithm minimizes the sum of squares deviations between data points and fitted functions. Conductivity data are fitted on a log K scale, because otherwise the large conductivity data would completely dominate the fitting result. Fitting both data types simultaneously is a multi-objective problem, and improving the fit for the retention data sometimes can be only accomplished by a worse fit for the conductivity data, and vice versa. The balance between fitting accuracy for the retention data and the conductivity data is specified by default with a stronger weight for the retention data, but the parameters can be modified by power users to any desired weighting scheme (see section 4.4.5).

4.4.2 Selecting a model and specifying parameter bounds

A hydraulic model is selected by marking the respective tick box. Permissible combinations of retention + conductivity models are highlighted; combinations that are not allowed are greyed.
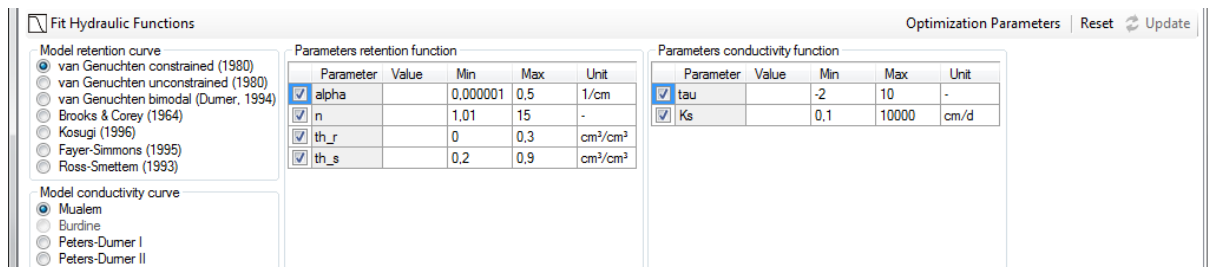
By default, all model parameters are included in the fitting process, and allowed to vary within a predefined range. The ranges of values are wide enough to cover physically consistent parameter combinations. A user can alter the permissible values of the bandwidths, by changing the default minimum and maximum value, but for most soils, this will not be necessary. An example for an exception would be fitting a retention curve of mosses, where water contents reach almost 100%. This may require you to set a higher value for the maximum saturated water content. In other cases, users may have prior knowledge about parameters that can lead to much reduced bandwidths.

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[1] In cases where the fitting will apparently not lead to a stop, the user can cancel the process from the Windows Task Manager.

Changing the default values for the minimum and maximum parameter values is done by typing the new value into the respective field in the group "Parameters retention function" and "Parameters conductivity function". To store a typed value, the cursor must be positioned out of the field, which can be done by pressing the "Tab" or "Return" key or by moving the mouse to another field.

If a hydraulic parameter should be kept at a pre-defined value, the tick-box in front of the respective parameter must be de-selected. In that case the fixed value must be inserted into the otherwise empty field. NOTE: For the decimal separator (i.e., appropriate use of comma or dot in the inserted numbers), the regional conventions of the Windows system is used.

If a model selection is changed, all specified parameter values will be automatically reset, i.e., by default all parameters are allowed to vary.

4.4.3 Results of the parameter estimation and uncertainty measures
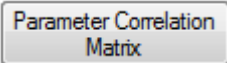
After termination of the fitting process, the appearance of the parameter fields switches from the input mode to the results mode. In results mode, the optimized parameters are shown in the previously empty column with the "Value" fields, and the uncertainties of the individual parameters are indicated by 95% confidence limits for the parameter values (expressed by the 2.5% quantiles and the 97.5% quantiles in the two following columns). For fixed parameters, the uncertainty is of course zero.

The quality of the fits is quantified in the group Statistical analysis in the upper right and can be visually inspected from the graphs (see section 4.4.4). Fit quality is given in terms of the root mean squares errors, separately calculated for the water content data and the log of conductivities. The root mean squares error (RMSE) is an indication of the mean distance between a data point and the fitted function. An RMSE of 0.001 for the retention data fit indicates an average distance of the fitted curve to observed data of 0.1 % water content. The effect of the parameter uncertainties on the uncertainties of the fitted functions can furthermore be visualized in the graphs by a grey-shading of the uncertainty bands. This option is only available for Power Users by selection the respective option in the Optimization Parameters menu (see section 4.4.5).

Models with a higher number of parameters are generally more flexible; hence the fitting error will become smaller for models with a larger number of parameters. This is counterbalanced by a higher correlation between the optimized parameters and higher uncertainties for the individual parameters.

Pressing the button Parameter Correlation Matrix will cause the pop-up of the parameter correlation matrix.

Correlation Matrix

	alpha	n	th_r	th_s	tau	Ks
▶ alpha	1,000	-0,649	-0,339	0,836	0,017	0,332
n	-0,649	1,000	0,895	-0,446	-0,019	-0,234
th_r	-0,339	0,895	1,000	-0,274	-0,015	-0,134
th_s	0,836	-0,446	-0,274	1,000	0,013	0,275
tau	0,017	-0,019	-0,015	0,013	1,000	0,872
Ks	0,332	-0,234	-0,134	0,275	0,872	1,000

In this symmetric matrix, the linear correlation coefficients of the parameters are listed. Negative values indicate that the increase of one parameter value can be (partly) balanced by a decrease of the other; positive values mean that an increase of either parameter value has a similar effect on the overall fit of the functions. Generally, correlation coefficients with absolute values smaller than 0.95 are not problematic and indicate a well-posed fitting problem. Too-high correlation of parameters is undesirable, since it indicates an over-parameterization of the selected model.

As an aid in deciding which model choice is most appropriate, HYPROP-DES shows in the Statistical analysis field additionally the corrected Akaike Information Criterion (AICc, Akaike, 1974). This criterion accounts for the different number of adjustable parameters when selecting the best model. The value will be normally negative. The smaller the value (i.e., the larger the absolute number), the more appropriate is the model. For details on the statistical criteria, see Peters and Durner (2008).

4.4.4 The function graphs
In the lower part of the "Fitting" register window, graphs with the calculated HYPROP data, the added data, and the fitted hydraulic functions are shown. The individual graphs can be switched on or off by pressing the respective buttons that are immediately above the graphs, to the left. Switching off a graph will resize the remaining graphs.

As with any other graphs in the HYPRO-DES software, the graphs can be magnified to full screen, or zoomed, by selecting the respective option in the context-sensitive submenu, which is activated by a right mouse click.

The fitted functions will disappear from screen if either parameter settings are changed (e.g., by modifying the permissible data range), or a setting in another register is changed that affects the calculated HYPROP data. After the fitting process, the fitting results can be exported in a variety of ways and graphs, which is specified in the final register »Export«.

4.4.3 Modifying optimization parameters (Power User only)
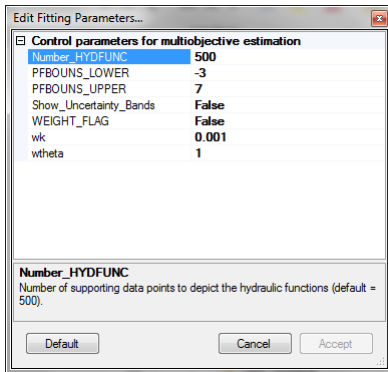
Power Users can edit some of the parameters that specify the calculations and the depiction of the fitted functions. The specifications are listed in the menu "Optimization Parameters" and described below.

Para-meter	Description	Default value	Public User can change value	Power User can change value
Number_HYDFUNC	The hydraulic functions in the graphs are taken from internal tables, where the functions are listed in the range PFBOUNS_LOWER to PFBOUNS_UPPER at discrete supporting points. Number_HYDFUNC is the number of supporting data points to depict the hydraulic functions.	500	No	Yes
PFBOUNS_LOWER	Lower bound for internal table of hydraulic functions, expressed as pF (=$\log_{10}(h)$ with h in cm). The default value expresses a minimum tension of 0.001 cm.	-3	No	Yes
PFBOUNS_UPPER	Upper bound for internal table of hydraulic functions, expressed as pF (=$\log_{10}(h)$ with h in cm). The default value is pF = 7, which is a tension of 10,000,000 cm.	7	No	Yes
Show_Uncertainty _Bands	Flag for showing the 95% uncertainty bands for the fitted functions in the depicted graphs by a grey shading.	False	No	Yes
WEIGHT_FLAG	The simultaneous fit hydraulic functions to retention data and conductivity data is a multi-objective minimization problem, which requires weights for the data of the different data types. HYPROP-DES provides the possibility to either pre-scribe these weights (WEIGHT_FLAG = False), or else to let the software iteratively balance out the weights in a way that both data sources (retention points and conductivity points) contribute in the same order of magnitude to the total fitting error (WEIGHT_FLAG = True). Since the retention data are normally better determined and cover a wider moisture range, we recommend to use the default values, where the weighting of the conductivity data is enhanced by a factor of 10^3.	False	No	Yes

wk	Weight of the conductivity data class. Default = 0.001, if WEIGHT_FLAG = false.	0.001	No	Yes
wtheta	Weight of the retention data class. Default = 1.0, if WEIGHT_FLAG = false.	1.0	No	Yes

4.5 Register "Export" - Exporting data, graphs, functions, and parameters
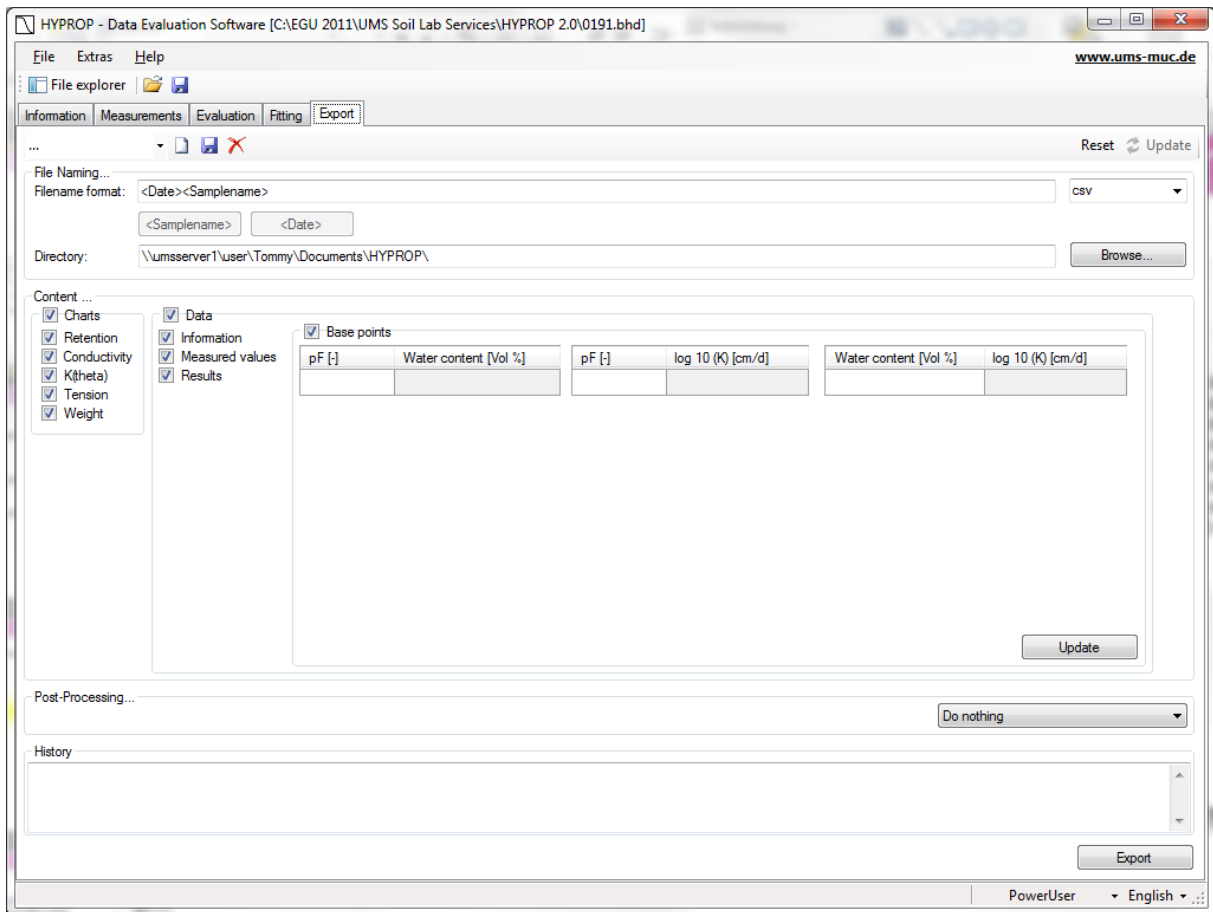
The register "Export" allows the simple export of all graphs, raw data, calculated data, fitted functions, and other parameters of interest.

HYPROP DES supports the following output formats:

csv   comma-separated values

csv(simple)   comma-separated values for re-import into HYPROP DES software

xls   Microsoft Excel file format

xlsx   Microsoft Excel file format

HYDRUS Table   HYDRUS Import file format

Different output settings are available and described below. The exporting is executed by clicking the button "Export".

File Naming…

Filename format

Enter the output file name in the field „Filename format". All permitted characters can be used in the filename.

The two default settings <Date> and <Samplename> are available for optional use in any position within the filename. They will automatically be replaced by the current date or sample name.

File format
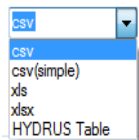
Select different file formats in the pull down menu.

Directory

Enter the output directory in the field "Directory" or click on „Browse" to select a directory.

Content

In the group "Content" you can select check boxes for the data that should be exported, and enter the base points for export.

In the group "Diagrams" you can select check boxes for the diagrams that should be exported.

In the group "Data" you can set the options for exporting raw data, calculated values and fitted functions.

Furthermore, you can enter freely definable base points for which the correlating data points then are calculated. To do so, enter the desired value in the table and the correlating data points are automatically calculated and exported when exporting is executed. Click "Update" to update the data points in the table.

Post- Processing…
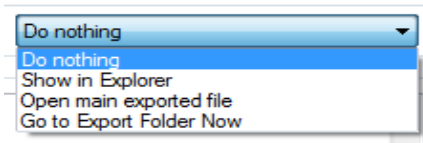
In the group "Post-Processing" you can set different actions that should be executed either after the exporting, or immediately.

History
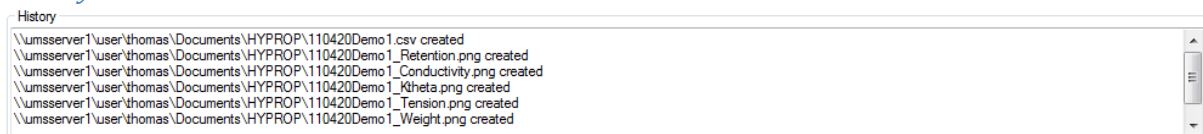
The group "History" gives an overview of all recently executed exports.

5. Processing multiple data sets
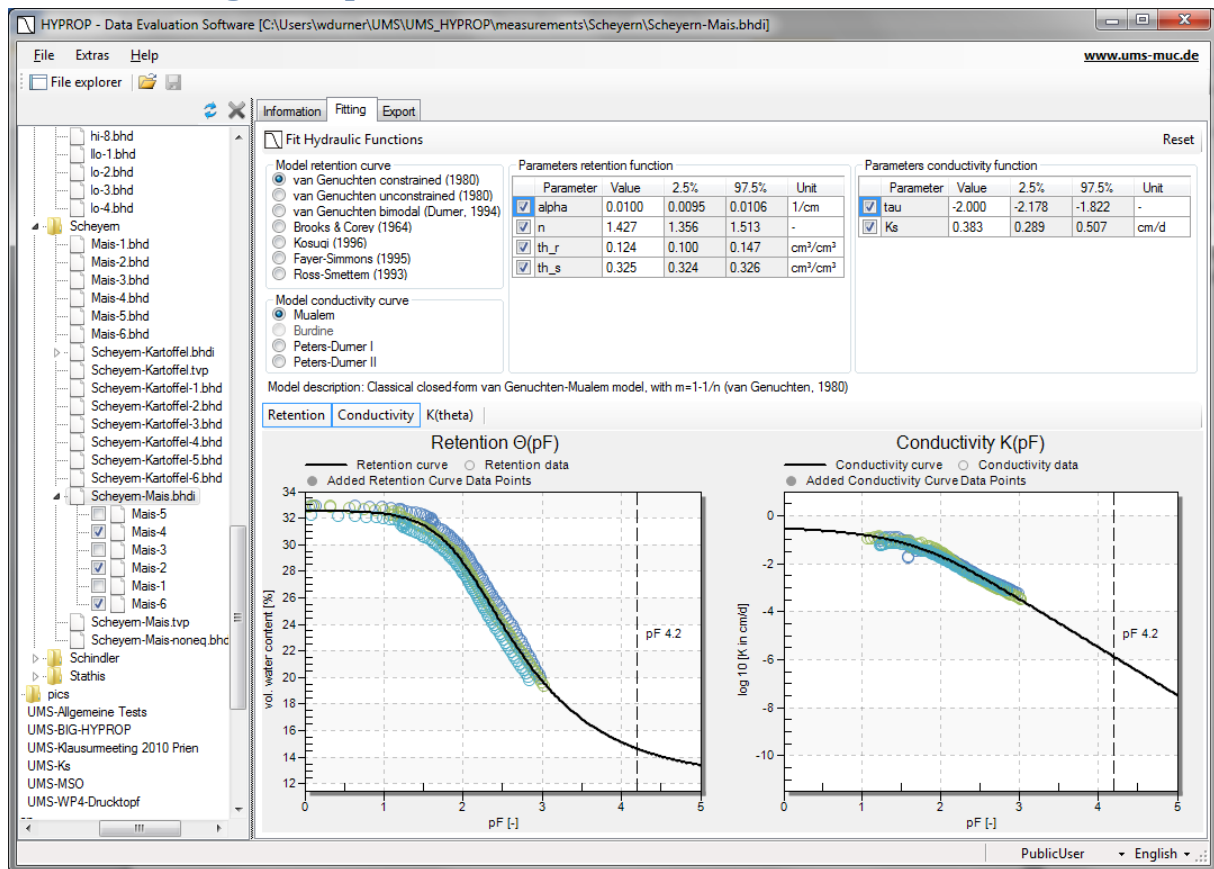
HYPROP-DES offers the convenient and powerful option to assemble individual data sets to combined data sets in so-called HYPROP binary iteration projects (files with extension *.bhdi). This is of particular use if data sets are to be compared, or if multiple data sets are to be fitted with a single hydraulic function.

The process to combine the individual .bhd files to a *.bhdi project is described the "Extras" Command menu, section 3.2.3. Once individual measurement campaigns are combined, they can be activated and de-activated simply by clicking on the individual tick boxes in the file explorer. As an example, in the figure above the measurement campaigns entitled Mais-1" to "Mais-6" are combined, but only three out of six campaigns are actually activated.

Data from different campaigns are shown in different colors. Fitting of functions occurs simultaneously for all depicted data.

Individual data sets can be fully edited and processed by single-clicking on the respective campaign name in the file explorer. The source file for the data will be unaffected, i.e., the .bhdi file contains copies of the original data. Clicking on the .bhdi name will return to the combined project menu, as shown above.

6. References

Akaike, H. (1974): A new look at statistical model identification, IEEE Trans. Autom. Control, AC-19, 716–723.

Peters, A., and W. Durner (2006): Improved estimation of soil water retention characteristics from hydrostatic column experiments, Water Resour. Res.,42, W11401, doi:10.1029/2006WR004952.

Peters, A. and W. Durner (2008a): Simplified Evaporation Method for Determining Soil Hydraulic Properties, Journal of Hydrology 356, 147– 162, doi:10.1016/j.jhydrol.2008.04.016

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Appendix 1 - Theoretical basics

Evaporation method (overview)

In a soil sampling ring two tensiometers, comparable to the T5 model, are installed in two depths (z_1 and z_2). The middle between the sensing tips of the tensiometers is the center of the soil sample. The sample is saturated, closed on the bottom and placed on a scale. The upper side of the sample is open to atmosphere so the soil moisture can evaporate. With the soil water tension [kPa] the average matric potential and the hydraulic gradient is calculated. The mass difference, measured by the scale, is used to calculate the volumetric water content and the water's flow rate.

A measuring campaign will last until one of the tensiometers runs dry or the mass changes become marginal. Then, the remaining moisture content is determined by oven drying the sample at 105°C for 24 hours. With these values the retention curve and the unsaturated conductivity is extrapolated.

Discrete data for retention and conductivity relation

At different points of time t^i the water tensions h_1^i and h_2^i (in hPa) of both depths are measured as well as the weight of the sample (in grams $\cong$ cm^3). The analytic procedure is based on the assumption that water tension and water content distribute linearly through the column, and that water tension and sample weight changes are linear between two evaluation points.

The initial water content is determined from the total loss of water (i. e. evaporation + water loss by oven drying). The average water content $\bar{\theta}^i$, derived from initial water content and loss of weight and the medial water tension $\bar{h}^i$ give a discrete value $\bar{\theta}^i(\bar{h}^i)$ of the retention function at any time t^i. For the calculation of the conductivity function it is assumed that between two time points t^{i-1} and t^i the water flow through the cross section situated exactly between both Tensiometers (and therefore exactly at column centre) is $q^i = \frac{1}{2}\left(\Delta V^i / \Delta t^i A\right)$. ΔV^i is the water loss in cm³ determined by weight changes, Δt^i is the interval between two evaluation points, and A the cross section area (in cm²) of the column.

The data for the hydraulic conductivity function are determined by inverting the Darcy-Equation:

$$K^i(\bar{\bar{h}}^i) = -\frac{q^i}{\left(\Delta h^i / \Delta z\right)+1}.$$

$\bar{\bar{h}}^i = \frac{1}{4}\left(h_1^{i-1} + h_2^{i-1} + h_1^i + h_2^i\right)$ is the medial water tension between two evaluation points, with K^i as the related hydraulic conductivity (in cm h^{-1}). $\Delta h^i = \frac{1}{2}\left((h_2^{i-1} - h_1^{i-1}) + (h_2^i - h_1^i)\right)$ is the medial difference of the water tension between both tensiometers, whereas $\Delta z = z_2 - z_1$ is the distance between both tensiometers (in cm).

Unreliable $K(h)$ data sets close to saturation are filtered depending to the measuring accuracy of the tensiometers. To get a sufficient number of data points for the hydraulic function even with relatively long intervals, both the tension curve and the weight curve between two evaluation points are interpolated with Hermitian splines (Peters and Durner, 2008). On this basis relatively short evaluation intervals are achieved.

Appendix 2 –Automatic estimation of the initial water content

After a measurement campaign, the initial water content is determined precisely from subtracting all tare weights from the total mass of the measuring assembly, i.e., by subtracting the tare weight of sensor unit, the mass of the sampling ring, and the mass of the dry soil, obtained after 24 hours drying at 105°C. If this value is not yet available, a guess of the initial water content can be obtained using the HYPROP-DES software by

$$\theta_s = 1 - \frac{m_0 - \rho_w \cdot V_{tot}}{(\rho_s - \rho_w) \cdot V_{tot}}$$

where θ_s (cm³ cm^{-3}) is the saturated volumetric water content, equal to the porosity and assumed to be the initial water content, ρ_w (g cm^{-3}) is the density of water, taken to be 1.0 g cm^{-3}, ρ_s (g cm^{-3}) is the density of the soil matrix, V_{tot} (cm^3) is the volume of the soil sample, and m_0 (g) is the mass of water plus soil at the beginning of the experiment, i.e., at full saturation. The value is taken from the total recorded weight at the start line, whereas all other values are as specified in the "Information" register.

Please note that this calculation assumes that all pores are water filled, so that the porosity is equal to the saturated water content. Since this is rarely the case in real evaporation measurements, this approximation is only a reasonable initial guess. An accurate calculation requires weighing the dry soil and inserting the respective value in the menu "Calculation of water contents" in the register "Evaluation".

Appendix 3 – Equations of the used retention and conductivity models

HYPROP-DES provides the choice of seven retention function models and four conductivity function models.

The retention functions
In all retention functions, the water content is expressed through the *Effective Saturation*, S_e, given by

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

where θ [cm³ cm^{-3}] is the volumetric water content, θ_r is the residual water content, and θ_s is the saturated water content. The retention functions are:

1. The unimodal constrained model of van Genuchten (1980)

$$S_e(h) = \left[\frac{1}{1 + (\alpha|h|)^n}\right]^{1-\frac{1}{n}}$$

where α [cm^{-1}] indicates a shape parameter that is related to the inverse of the air-entry pressure, and *n* [-] is a shape parameter that controls both the bending of the retention curve at the air-entry region and the asymptotic curvature towards the residual water content.

With four free parameters, the constrained van Genuchten (1980) function is the most widely used expression to describe water retention data in vadose zone hydrology. It fits retention data with a unimodal shape, a gradual air entry, and an asymptotic approximation of a finite residual water content. Despite its wide use, the model has deficiencies if used for natural soils with structured pore systems, and for describing data that encompass a wide pressure head range and approximate smaller water contents towards dryness.

2. The unimodal unconstrained model of van Genuchten (1980)

$$S_e(h) = \left[\frac{1}{1 + (\alpha|h|)^n}\right]^{m}$$

where *m* [-] is an additional free shape parameter. In this five-parameter function, *n* determines primarily the bending of the retention curve around the air-entry region, whereas the product of *n·m* determines the curvature towards the residual water content. In essence, the unconstrained model of van Genuchten is more flexible and encompasses arbitrarily sharp air-entry regions, with the Brooks & Corexy function as a limiting case with $n\rightarrow\infty$, $m\rightarrow0$ and $n·m\rightarrow\lambda$ (see model 4). Despite its higher flexibility, the five-parameter van Genuchten model is less often used than the constrained form, because its combination with the Mualem (1976) conductivity model does not yield a closed-form expression for the combined conductivity function (see next section).

3. The bimodal van Genuchten model of Durner (1994)

$$S_e(h) = \sum_{i=1}^{2} w_i \left[\frac{1}{1 + (\alpha_i |h|)^{n_i}} \right]^{1 - \frac{1}{n_i}}$$

This model is a weighted superposition of two van Genuchten functions, where the weights w_1 [-] and w_2 [-] add up to unity, $w_1 + w_2 = 1$. Each of the subfunctions has now its own shape factors α_i [cm^{-1}] and n_i [-]. This seven-parameter function is much better suitable than the unimodal models to describe the retention functions of structured soils, but due to its overall flexibility it is also better suited to fit data of loamy or sandy soils that just do not follow perfectly the van Genuchten unimodal shape. Priesack and Durner (2006) showed that the combination of this bimodal model with the Mualem (1976) conductivity model yields a closed-form expression for the combined conductivity function (see next section).

4. The model of Brooks and Corey (1964)

$$S_e(h) = \begin{cases} (\alpha\,|h|)^{-\lambda} & \text{for} \quad (\alpha\,|h|) > 1 \\ 1 & \text{for} \quad (\alpha\,|h|) \leq 1 \end{cases}$$

is a model that was traditionally widely used in the geosciences. Similar to the constrained van Genuchten model, it is a four-parameter model with λ expressing the width of the pore-size distribution. The model is particularly suitable for soils with a very sharp air-entry point. It is traditionally combined with the Burdine (1953) conductivity model, whereas the other six model in the HYPROP-DES suite are combined with the Mualem model.

5. The model of Kosugi (1996) is given by

$$S_e = Q\left[\frac{\ln(h/h_m)}{\sigma} \right]$$

where Q indicates the integral of the Gaussian normal distribution, h_m [cm] is the pressure head at the pore-density maximum, and σ [-] indicates the standard deviation of the pore-size density distribution. The flexibility and overall shape of this four parameter model is very similar to the constrained van Genuchten model, but some users prefer it due to a more straightforward statistical interpretation of its parameters. A certain disadvantage is that the integral of the normal distribution is not a simple algebraic expression.

6. The Fayer and Simmons (1995) model: Shiozawa and Campbell (1989) introduced an extension for water retention curves that describes an exponential decrease of the water content towards total dryness at pF 6.9, i.e., gives a simple straight line expression on a θ-pF scale. Fayer and Simmons (1995) combined this approach with the van Genuchten model, leading to

$$\theta(h) = \theta_r(h) + [\theta_s - \theta_r(h)] \left[\frac{1}{1 + (\alpha|h|)^n} \right]^{1 - \frac{1}{n}}$$

with

$$\theta_r(h) = \theta_a \left(1 - \frac{pF}{6.9} \right)$$

where the parameter θ_a is specified instead of the residual water content. Whereas θ_s is a constant parameter in the original van Genuchten formulation, it becomes now a function of h that reaches 0 at pF 6.9.

7. The model of Ross and Smettem (1993)

$$S_e(h) = (1 - w_2) \frac{1 + \alpha_1 |h|}{e^{-\alpha_1 |h|}} + w_2 \left[\frac{1}{1 + (\alpha_2 |h|)^n} \right]^{1 - \frac{1}{n}}$$

The Ross-Smettem model is a model for soils with bimodal pore-size distributions. It is slightly less flexible than the Durner model, due to one less free parameter, but might fit some observed data very well.

The conductivity functions

Combinations with traditional pore-bundle predictive models

The seven retention models are coupled with corresponding conductivity models by plugging those into the capillary pore-bundle model of Mualem (1976). An exception which is kept for historical reasons is the Brooks and Corey retention function, which is traditionally combined with the capillary bundle model of Burdine (1953). The Mualem and the Burdine models predict the shape of the conductivity function from the shape of the retention function. Thus, shape parameters of the retention function determine the shape of the conductivity function, which is traditionally expressed by the relative conductivity, $K_r(h)$,

$$K(h) = K_s \cdot K_r(h)$$

Mualem's predictive model for K_r is given by

$$K_r(S_e(h)) = S_e^\tau \left[\frac{\int_0^{S_e} h^{-1} dS_e(h)}{\int_0^1 h^{-1} dS_e(h)} \right]^2$$

where τ is an additional fitting parameter, called tortuosity parameter, which is often set to $\tau = 0.5$, but must be regarded as pure optimization parameter (Hoffmann-Riem et al., 1999). Plugging the retention curve expression $h(\theta)$ of the constrained van Genuchten function into the integral yields a closed-form expression for $K(h)$ (van Genuchten, 1980), which is probably the primary reason for the popularity of the van Genuchten/Mualem model:

$$K(h) = K_s (1 + (\alpha |h|)^n)^{\tau(1/n-1)} \left[1 - (\alpha |h|)^{n-1} \left[1 + (\alpha |h|)^n \right]^{1/n-1} \right]^2$$

.

The Mualem model can be combined with any of the retention models, but not all lead to closed form functions. The combination of the bimodal Durner retention function with Mualem's K-model yields (Priesack and Durner, 2006)

$$K(h) = K_s \left[\sum_{j=1}^2 w_j \left[1 + (\alpha_j |h|)^{n_j} \right]^{1/n_j - 1} \right]^\tau \left[\frac{\sum_{j=1}^2 w_j \, \alpha_j \, \{1 - (\alpha_j |h|)^{n_j - 1} [1 + (\alpha_j |h|)^{n_j}]^{1/n_j - 1}\}}{\sum_{j=1}^2 w_j \alpha_j} \right]^2,$$

where j are indices for the parameters of each van Genuchten function, and w_j are the weights of both partial functions. The following restriction applies: $0 < w_j < 1$ and $\sum w_j = 1$.

The combinations of the other retention curve models with the Mualem models lead to conductivity functions that are calculated in HYPROP by numerical integration.

Based on similar capillary bundle considerations as the Mualem model, the combination of the Brooks & Corey retention function with the Burdine conductivity model gives (Brooks and Corey, 1964):

$$K(h) = \begin{cases} K_s & \text{for} \quad h \geq \alpha^{-1} \\ K_s \left[(\alpha|h|)^{-\lambda} \right]^{2/\lambda+\tau+2} & \text{for} \quad h < \alpha^{-1} \end{cases}$$

As for the Mualem model, the slope of the conductivity function vs. pF is determined by the pore-size distribution parameter of the retention function, and additionally by a tortuosity parameter τ [-], which is regarded as fitting parameter.

Combinations with conductivity prediction models including film flow

The commonly used models for characterizing hydraulic conductivity of porous media rely on pore bundle concepts that account for capillary flow only and neglect film flow. Experimental evidence suggests that water flow at medium to low water contents in unsaturated porous media can be significantly underestimated by these capillary bundle models. Peters and Durner (2008b) introduced a new model that combines a film flow function, expressed by a simple power function of effective saturation, with the capillary flow model of Mualem. This new model can easily be coupled to any water retention function. Moreover, due to its mathematical simplicity, it can easily and efficiently be implemented in existing codes for the numerical solution of unsaturated flow problems.

The new model was introduced in a constrained and an unconstrained version. The constrained version (Peters-Durner I) is given by

$$K_r(S_e(h)) = (1 - \omega) S_e^\tau \left[\frac{\int_0^{S_e} h^{-1} dS_e(h)}{\int_0^1 h^{-1} dS_e(h)} \right]^2 + \omega S_e^\tau$$

where ω is one additional parameter, as compared to the original Mualem model, which expresses as weighing factor the contribution of the film flow component to the total conductivity. The unconstrained version (Peters-Durner II) increases the flexibility of the model by an additional parameter τ_2 [-] for the film-flow part

$$K_r(S_e(h)) = (1 - \omega)S_e^{\tau 1} \left[\frac{\int_0^{S_e} h^{-1} dS_e(h)}{\int_0^1 h^{-1} dS_e(h)} \right]^2 + \omega S_e^{\tau 2}$$

Peters and Durner (2008b) investigated a set of soil water retention and conductivity data from the literature that all reached dry conditions and were poorly described by existing capillary bundle models. These data were well described with the new model if the model was coupled with an appropriate retention function. Investigation of conductivity data from the UNsaturated SOil hydraulic DAtabase (UNSODA) database showed that, in 75% of all data sets, the new model achieved the best performance using a modified version of Akaike's information criterion.

Parameter Optimization with Integral Fit

The $\theta(h)$ and $K(h)$ functions are adapted simultaneously to the data points. This is essential as distinct parameters (e.g., α and n for van Genuchten/Mualem model) influence the shape of both functions. The adaption is accomplished by a non-linear regression under minimization of the sum of all assessed squares of the distance between data points and model forecast. Since the assumption that the water content is spread out linearly over the column is not always fulfilled in coarse pored or structured soil, the so called "integral fit" is applied for the adaption of the retention function to avoid any systematic error (Peters and Durner, 2006). For details of the fitting procedure and data assessment please refer to Peters and Durner (2008a).

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