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# 1. INTRODUCTION

Thank you for choosing the HYPROP® 2 automated measuring and evaluation system to determine the hydraulic properties of soil samples from METER Group.

This user manual covers the operation of the LABROS SoilView-Analysis software. It is a tool used to evaluate measurements obtained using the Simplified Evaporation Method (SEM) function in the HYPROP 2. It should be read along with the HYPROP 2 User Manual (metergroup.com/en/meter-environment/products/hyprop-2/hyprop-2-support). This document includes detailed information about using HYPROP 2 Data Evaluation Software (LABROS SoilView-Analysis) and provides scientific background related to the function of the HYPROP 2. LABROS SoilView-Analysis is also available for download at (metergroup. com/products/hyprop2-support). This software is also available for evaluating VARIOS measurements.

# 2. OVERVIEW AND SCIENTIFIC BACKGROUND

LABROS SoilView is compatible with Microsoft® Windows® 10 or newer. The software reads data that is recorded in HYPROP 2 projects using the data acquisition software LABROS SoilView and stored as \*.bhdx files. Separate data sets consisting of measured retention (e.g., from a WP4C) and conductivity data (e.g., from a KSAT) can be imported and fitted.

LABROS SoilView-Analysis performs the following operations:

- Specifies parameters for the evaluation of recorded experimental data with SEM, such as column length, tensiometer positions, tare weights of the measurement device components, steel rings used, etc.
- Creates visual images of the raw data, such as tensions, weight changes, and specification of start and stop points for the data evaluation.
- Recalculates tensions and net weight data as a base for the retention and conductivity data calculation. This includes temporal interpolation for data in low-temporal resolution and aggregation of data in very high-temporal resolution.
- Calculates and visualizes data for retention and conductivity characteristics.
- Fits state-of-the-art hydraulic functions to the data; visualizes functions, and lists hydraulic parameter values and confidence limits.
- Exports graphs, raw data, calculated data, fitted functions, and other parameters of interest.

HYPROP 2 measurement campaigns follow the SEM method. This method uses soil sample weight changes and matric potential measurements during a drying process caused by evaporation to derive soil hydraulic functions. The principles of the SEM method were first formulated by Wind (1968). A simplification of the SEM method, which is implemented in HYPROP 2 measurements, was proposed by Schindler (1980). Further advancements of the SEM method are included in the LABROS SoilView-Analysis software, 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 SEM method has been investigated by Peters and Durner (2008) and Peters et al. (2015). The detailed implementation of the method in the LABROS SoilView-Analysis software follows the descriptions given in these papers. 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 of the validity range of conductivity data in the range near saturation, where the hydraulic gradient becomes too small to yield reliable data. The SEM method yields correct results for soils where the water flow is validly described by the Richards equation with time-invariant hydraulic properties, and with hydraulic properties that can be described with parametric expressions, including isothermal vapour diffusion (Peters et al., 2015). For further information about the scientific background of the method, the reader is referred to the scientific publications listed in the references section.

# 3. OPERATION

Please read all instructions in this section before operating the LABROS SoilView-Analysis software to ensure it performs to its full potential.

# INSTALLATION

Use the following instructions to install the LABROS SoilView-Analysis software on a laptop or Windows PC.

NOTE: The LABROS SoilView-Analysis software is only compatible with Windows 10 or newer. It will not run on a Mac.

- 1. Navigate to the METER Environment downloads webpage (meter.ly/software-downloads).
- Click on the LABROS SOILVIEW-ANALYSIS SOFTWARE DOWNLOAD link.
   The LABROSSoilView vx.x.x.exe file will be downloaded to the Downloads folder.
- Double click on the LABROSSoilView\_vx.x.x.exe file to start the installation
   NOTE: If there is a problem executing the file HYPROP\_vx.x.x.exe, please download and install Microsoft.NET Framework 4.8 manually, and be sure to have the current version of the Windows installer.
- 4. Click the **Next** button in the lower right corner of the HYPROP Setup window.
  - a. To install both LABROS SoilView and LABROS SoilView-Analysis software click on the **DEFAULT** button to use the default installation settings (Figure 1).
  - b. To install either LABROS SoilView-Analysis software, do the following (Figure 1):
    - i. Click on the DOWN ARROW next to the software that should NOT be installed.
    - Select the Entire feature will be unavailable in the dropdown list window that appears.
    - iii. Click on the NEXT button to start the installation This will keep the selected feature from being installed.

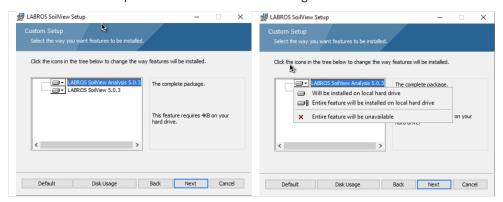


Figure 1 Custom Setup screens

5. Following the instructions in the installation wizard window until installation is complete.

# 3.1 ACCESS RIGHTS

LABROS SoilView-Analysis can be run in two different user modes affecting the permissions to write or change parameters. The user mode is depicted in the bottom line on the right of the software window.

### 3.1.1 PUBLIC USER MODE

In public user mode the software runs in a standard manner and default values are applied for most specifications.

To change the user mode, select the appropriate mode from a drop-down menu located in the lower right corner of the screen. A change of user status can be done at any time and from any register. The change will be active immediately.

## 3.1.2 POWER USER MODE

Power user mode should only be used by experienced and skilled users who are trained in soil physics and are familiar with the scientific background of data processing. Power user mode allows the user to alter many of the default values or manipulate measurement data.

# Example

In power user mode, the user can edit or delete measured data records that are obvious outliers, or they can delete undesired records at the beginning or end of a measurement campaign.

Furthermore, they 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.

# 3.2 STARTING THE PROGRAM

To start the LABROS SoilView-Analysis software do the following:

- 1. Open the Windows Start menu.
- Select LABROS SoilView-Analysis (or LABROS SoilView) from the list of programs.
   On the first start of the software, a welcome screen will appear (Figure 2). The welcomes

On the first start of the software, a welcome screen will appear (Figure 2). The welcome window shows three header lines:



Figure 2 Welcome screen header lines

NOTE: The Feedback button can be used for sending a feature request, a bug report, a question, or other comments. Please be sure to enter a correct email address for contact.

A list of all new features and bug fixes included in the current version are listed (Figure 3). For more information about updates, the user can do one of the following options to view a PDF file.

- Select the two arrows (>>) at the end of each item to open a PDF with more detail.
- Select the Help menu item on the second header line and What is New from the dropdown list.

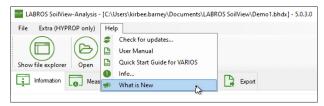


Figure 3 What is new screen

If data sets had been loaded in a previous session, LABROS SoilView-Analysis will automatically load the data set that was used last. However, if the last exit from the software was not regular (e.g., a crash caused by a corrupted data file), the software will open with an empty screen and data sets will have to be reloaded.

# 4. PROJECTS

The information below describes the software menus and how to set up HYPROP projects.

# 4.1 OVERVIEW

All commands follow the standard Windows operating system conventions used in Windows graphical user interfaces (GUI).

The Show/Hide file explorer icon in the third header line acts as a toggle that opens and closes a file explorer window on the left side of the main window (Figure 4).



Figure 4 Show/Hide toggle command

The Save icon opens a Save window enabling the user to name the file and choose where the file will be saved. Command icons or entries that cannot be actively selected in a certain situation are shown in grey and cannot be used. For example, the Save icon can only be used if a project has been opened and modified (Figure 5).



Figure 5 Save, Save as command

A list of more possible actions associated with the menu item or icon is indicated by a vertical triangle on the right side of the respective icon or entry (Figure 6).

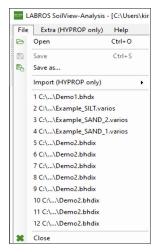


Figure 6 List of additional command actions

Entries can sometimes be selected by key-combinations. If so, the combinations are indicated to the right of the respective entry. To return to a previous menu or action, press the **ESC** button.

The following types of data can be processed in the LABROS SoilView- Analysis software:

- HYPROP binary project (\*.bhdx)
- HYPROP binary iteration project (\*.bhdix)
- ASCII files (\*\_config.csv) with a predefined data structure
- Separately measured retention and conductivity data in ASCII files (\*\_RETC.csv and \*\_COND.csv), stored in a \*.fitx project file
- Raw data from tensioVIEW measurement campaigns (\*.tvp) performed with the HYPROP experimental setup.

# 4.2 FILE MENU

The File menu is used to open and save project files, and to import retention and conductivity data measurements.

# 4.2.1 OPENING A PROJECT FILE

Assuming that an existing data file is available, open the project using the following instructions.

1. Select File from the menu on the second header line (Figure 7).

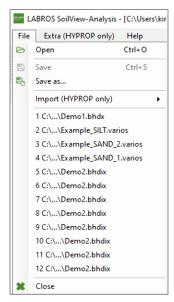


Figure 7 Select File

2. Select Open from the dropdown list (Figure 8).

The Open window, which looks like a file explorer window, will open.

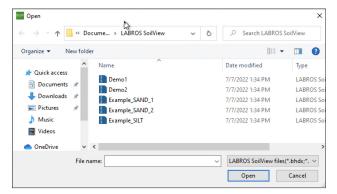


Figure 8 File > Open window

Select the desired file by navigating in the Open window to the desired folder (Figure 8).
 Only files with LABROS SoilView-Analysis compatible extensions will show in the Open window.

After opening a file, a fourth line with three to five tabs will appear. The tabs are titled Information, Measurements, Evaluation, Fitting, and Export (Figure 9).

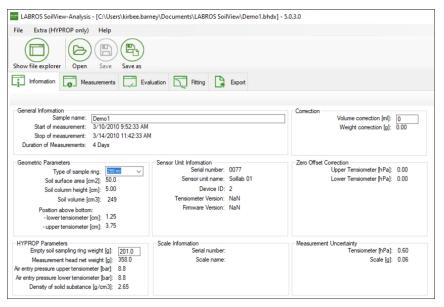


Figure 9 Open window

# 4.2.2 FILE MENU OPTION DEFINITIONS

The following subsections descript the file menu option definitions.

## 4.2.2.1 FILE > OPEN

The Open option is the first entry in the File menu. Table 1 describes the five types of data files that can be opened.

Table 1 Data Types Opened With File > Open

File Type	Description
*.bhdx (Default)	A LABROS SoilView-Analysis version 3.0 (or higher) and a LABROS SoilView-Analysis version 5.0 (or higher) binary project file containing information, measurement data, calculated conductivity and retention data, and fitted function for a single measurement campaign (also the HYPROP-FIT version 2.0 format, *.bhd, can be processed).
*.bhdix	A LABROS SoilView-Analysis version 3.0 (or higher) and a LABROS SoilView-Analysis version 5.0 (or higher) iteration project file, including data and fitted functions for multiple measurement campaigns (also the HYPROP-FIT version 2.0 format, *.bhdi, can be processed).

Table 1 Data Types Opened With File > Open (continued)

File Type	Description
*.fitx	Retention and conductivity data that were not collected with the HYPROP 2 system but saved as *.csv files with the endings *_retc.csv (including retention data) and *_cond.csv (including conductivity data).
*.tvp	TensioVIEW data files that have been produced by a HYPROP 2 measuring campaign and stored by the data acquisition system in a tensioVIEW project file (review the HYPROP 2 User Manual for more tensioVIEW information).

HYPROP-FIT version 2.0 (or higher) measurement files can be opened in LABROS SoilView-Analysis version 5.0 (or higher). Measurement files are not backward compatible.

If there is a dataset with more than 10,000 data points, the software will not be able to proceed with this file. By opening this file, the software automatically reduces the number of data points by deleting every third record. The reduced file will be saved automatically as a copy of the original file.

#### 4.2.2.2 FILE > SAVE

The Save option is used to save a project file that has been imported or processed. All changes will be saved in the folder under the name where it is already saved. If no changes to an existing project have been made, the Save icon/menu entry shows as a grey shade to indicate it is inactive.

#### 4.2.2.3 FILE > SAVE AS...

The Save As... option is used to save a file under a different name.

NOTE: A file can be opened and processed with LABROS SoilView-Analysis during the data acquisition stage. However, this original file is write-protected as long as the measurement campaign continues. If desired, the file can be saved with a different name.

#### 4.2.2.4 FILE > IMPORT

The Import function is used for HYPROP data sets that have been previously exported and edited outside the LABROS SoilView-Analysis software, and are now ready to be imported back into LABROS SoilView-Analysis format.

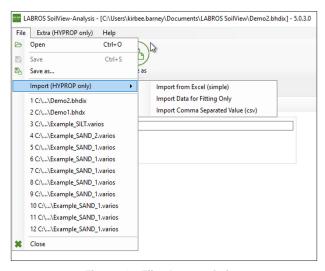


Figure 10 File > Import window

# There are three import options:

Import from Microsoft Excel® spreadsheet file (\*.xlsx).

If the \*.bhdx file was exported as an Excel spreadsheet file (\*.xlsx), it can be imported as an Excel.

Please maintain the format of the exported Excel (simple) spreadsheet file while editing:

- Heading names
- Tab names and sequences
- Column number
- Cell formats

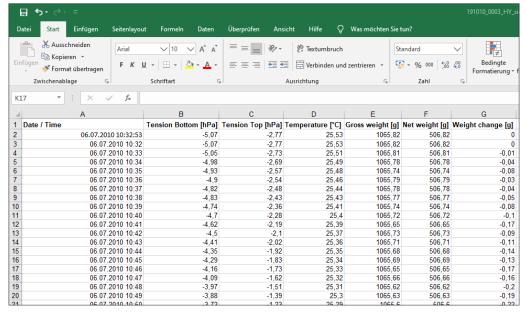


Figure 11 Example simple Excel spreadsheet

2. Import comma-delimited value (\*.csv)

If the \*.bhdx file was exported as \*.csv (simple), it can be imported as a \*.csv file.

During export the software creates three files: \*\_config.csv, \*\_weight.csv; \*\_tension.csv. Please keep the preset format while editing:

- Heading names
- Tab names and sequences
- Column numbers
- Cell formats
- Preset separation sign

For import, all three files (\*\_config.csv, \*\_weight.csv; \*\_tension.csv) have to be placed in the same folder. Be sure to keep the preset endings of the files. All information will be imported by selecting the \*\_config.csv file.

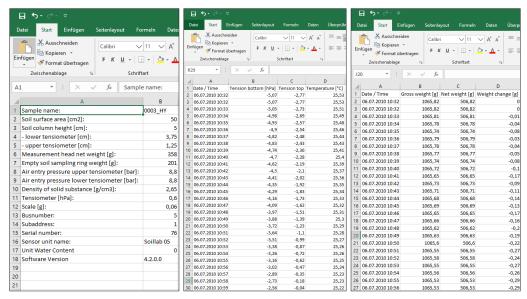


Figure 12 Imported comma-delimited files

## 3. Import Data for Fitting only.

It is also possible to import retention and conductivity data that were not collected with the HYPROP system. For this type of data, an Excel spreadsheet file has to be created that includes all needed data. This file must be saved as a \*.csv file with following endings: retc (including retention data) or cond (including conductivity data).

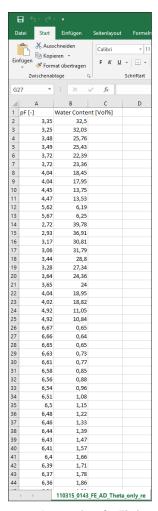


Figure 13 Import data for Fitting only

#### 4.2.2.5 RECENTLY OPENED PROJECT FILES

The group of entries below Import in the File menu are recently opened projects. This allows direct and quick access to these projects files by selecting the project filename.

#### 4.2.2.6 FILE > CLOSE

The Close option closes the data file. If changes have been made, a message window asking for confirmation to save changes or not will appear.

## 4.2.3 EXTRA MENU

The Extra menu item is used to do the following actions:

- Convert tensioVIEW project (\*.tvp) files...
- · Join files to an iteration file...
- Merge files to a single file...

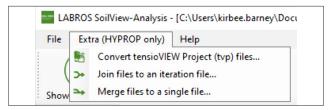


Figure 14 Extra menu window

## 4.2.3.1 CONVERT TENSIOVIEW PROJECT (\*.TVP) FILES...

This option is used to read existing tensioVIEW data files that have been produced by a HYPROP 2 measuring campaign and stored by the data acquisition system in a tensioVIEW project file. In the browser window that opens, navigate to the location of the files to be imported and select. The imported file will be immediately converted to one or more HYPROP binary data (\*.bhdx) files and can be stored and further processed.

#### 4.2.3.2 JOIN FILES TO AN ITERATION FILE...

This option is used to combine measuring campaigns that are stored as \*.bhdx files to one combined project file of type \*.bhdix. 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. Please find more information in Section 6.

#### 4.2.3.3 MERGE FILES TO A SINGLE FILE

This option is used to merge two or more files of one measurement. This option is useful if the software crashed during HYPROP 2 measurement (e.g., due to failure in power supply), and the measurement was restarted after a certain time. Two parts of one measurement can be combined again in one project by using this command.

## 4.2.4 HELP MENU—LABROS SOILVIEW-ANALYSIS VERSION INFORMATION



Figure 15 Extra menu window

#### 4.2.4.1 CHECK FOR UPDATES...

This option gives information about new available software versions and provides a download link if necessary.

#### 4.2.4.2 USER MANUAL

This option provides the current version of LABROS SoilView-Analysis manual as a PDF document for view, print, or download.

#### 4.2.4.3 INFO...

This option shows the used version of the HYPROP Data Evaluation Software (LABROS SoilView-Analysis), lists the HYPROP development team, and shows the disclaimer.

#### 4.2.4.4 WHAT IS NEW

This option shows a PDF file describing all new features and bug fixes coming with this software version.

# 5. THE REGISTERS—PROCESSING DATA



Figure 16 Registers

The LABROS SoilView-Analysis software groups the data processing in five registers (Figure 16) 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 by selecting the right user mode.

The following points are common to all registers:

- Editable values are shown in an 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 (Section 3.1).
- When inserting a numerical value, the proper decimal separator sign depends on the region settings of the computer. Default for the German Operating System is the comma, and default for the English one is a dot (period).
- Fields for numerical values do not accept input of alphabetical letters or special signs; if a user attempts to insert a nonpermitted character, the field does not show the typed character.
- To be sure that an input operation is saved, the cursor must leave the input field. This is
  achieved either by pressing the Tab key, the Return key, or by moving the cursor to another
  position in the window and clicking the left mouse button. In some menus an Accept button
  must be pressed.
- When placing the cursor over a button, information (Quickinfo) about the button function pops up for a period of a few seconds.
- Context-sensitive menus can be activated by right-clicking the mouse while the cursor hovers over some graphs and other content items.

# **5.1 INFORMATION REGISTER**

This section describes how to use the Information register to specify the required parameters for the measurement.

#### THE REGISTERS—PROCESSING DATA

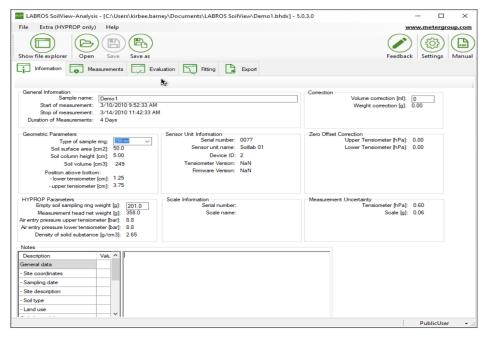


Figure 17 Information register

The Information Register (the first of five tabs) is a window that contains 10 blocks providing information about the selected project. Some of the data are editable by the Public User, and some data are editable only by the Power User. Other data cannot be altered by the user and are listed as information that is specified by the LABROS SoilView data acquisition program and the respective firmware.

In a typical measurement evaluation, there is one single input value that has to be specified by the user. This is the "Empty soil sampling ring weight" [g] in the group "HYPROP parameters". Since the sampling ring weight differs from sample to sample, the weight of the ring must be specified for each individual measurement. Without this value, an evaluation cannot be performed.

# 5.1.1 DATA GROUPS

The following paragraphs list and explain the data groups and inputs.

## **GENERAL INFORMATION DATA GROUP**

General Information

Sample name: 0026\_HY

Start of measurement: 29.06.2011 12:48:55 Stop of measurement: 07.07.2011 10:08:55

Duration of Measurements: 7 Days

Figure 18 General Information

# Table 2 Data Group—General Information

Falls builter					
			Editable	by User	
Variable	Explanation	Data Value	Public	Power	
Sample name	Denomination of a sample. The name can be chosen freely by the user. Note that the sample name is used for the creation of the file name during export by default. The file name rules, specified by Windows, have to be considered. If data stem from a HYPROP 2 measurement campaign with LABROS SoilView, the sample name specified in LABROS SoilView is listed here.	Sample name from LABROS SoilView	Yes	Yes	
Start of measurement	Date and time from the start of the recorded data. These data are given by the *.bhdx file.	_	No	No	
Stop of measuremen	Date and time from the end of the recorded data. These data are given by the *.bhdx file.	_	No	No	
Duration of measurement	Difference between start and end date of the recorded data, calculated from the two fields above and rounded to full days.	_	No	No	

#### CORRECTION DATA GROUP

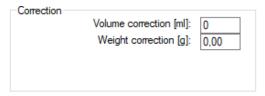


Figure 19 Correction

Table 3 Data Group—Correction

	I			
			Editable	by User
Variable	Explanation	Data Value	Public	Power
Volume correction	Correction of the sample volume. This can be necessary for example, if the prepared sample surface is not perfectly prepared and shows deficits (negative correction) or shows roughness. Volume correction will affect the calculation of the water contents since the weight changes will be related to the value volume plus volume correction.	0 cm³	Yes	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. In this case the additional weight value has to be entered as a positive value.	0 g	No	Yes

#### GEOMETRIC PARAMETERS DATA GROUP

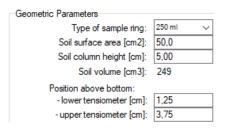


Figure 20 Geometric Parameters

Table 4 Data Group—Geometric Parameters

	Table 4 Data Group	deometricia	amotoro		
				Editable	by User
Variable	Explanation		Data Value	Public	Power
Type of sample ring	The sample ring can be chose 250 ml ring (standard METE ring) and 100 ml ring with 2-(standard sample ring to use 2-in adapter from METER). I already chose the used type ring in the LABROS SoilView the selected value is adopted.	R soil sample in adapter e with the f the user of sampling software,	250 ml	Yes No- Custom	Yes
	A customized sample ring ca chosen. Geometric paramet to be adjusted. Selecting the ring will affect the subseque entries for surface area and aware that the height ratio be column height and tensiome has to stay the same as for a standard sampling ring height of using a higher sample column tensiometer shaft must be a	ers have is sample ent default height. Be between soil ster height the METER ht (250 ml). umn, a higher			
Soil surface area	Shows the surface area of dependent on the chosen t sample ring.		50.0 cm <sup>2</sup>	No	Yes
Soil column height	Height of soil sample. Defau given by METER standard sa e.g. swelling occurred durin and the user decided not to saturated sample to exactly value has to be adapted.	ample rings. If g saturation cut the	5.0 cm	No	Yes
Soil volume	Volume of soil sample. It is of from the entries of area and corrected for the removed vitwo tensiometer candles (1 entered volume correction.	height, and olume for the	249.0 cm <sup>3</sup>	No	No
Position above bottom: lower tensiometer	Height level of the ceramic to tensiometer with the short some asured from the base of sample. Default value is valimeter HYPROP device, who tensiometer is located at on the total height.	shaft, the soil d for the ere the lower	1.25 cm	No	Yes
Position above bottom: upper tensiometer	Height level of the ceramic ti the tensiometer with the lon measured from the base of t sample. Default value for the HYPROP device is three-four sample height.	g shaft, he soil e METER	3.75 cm	No	Yes

#### SENSOR UNIT INFORMATION DATA GROUP



Figure 21 Sensor Unit Information

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

Table 5 Data Group—Sensor Unit Information

	·		Editable	byllear
			Euitable	by User
Variable	Explanation	Data Value	Public	Power
Serial number	Information given by METER firmware through *.bhdx file.	_	No	No
	NOTE: This number is always unique identification of the measurement device! Together with the date information, it is a unique identifier of the measurement.			
Sensor unit name	Information as specified in data acquisition and stored in the *.bhdx file.	_	No	No
Device ID	Information as given in the data acquisition and stored in the *.bhdx project file. Device ID can be modified in the LABROS SoilView data acquisition software. This can be necessary for the multi-head mode, for the seldom case that the default Device IDs of two measuring heads are the same.	_	No	No
Tensiometer Version	Information given by METER firmware.	_	No	No
Firmware Version	Information given by METER firmware.	_	No	No

## ZERO OFFSET CORRECTION DATA GROUP



Figure 22 Zero Offset Correction

An offset correction is required if the user has an indication from the measurement that the calibration of a tensiometer was not correct. In general, the tensiometers must show a difference of approximately 2.5 hPa under almost hydrostatic conditions, which prevail for most soils in the initial measurement phase. Deviations from this difference will strongly affect the calculation of the conductivity values at the wet end of the range. If a tensiometer time series appears shifted by an offset, it is possible to correct the whole data set for that shift by inserting the offset in the respective box. The correction will be directly applied to all recorded tensions (and accordingly visualized in the Measurement register, Figure 16).

WARNING: Be careful! Please correct tensions to assumed hydrostatic conditions only when sure that these conditions were actually given at a given time during the measurement campaign.

Table 6 Data Group—Zero Offset Correction

			Editable by User	
Variable	Explanation	Data Value	Public	Power
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

#### HYPROP PARAMETERS DATA GROUP

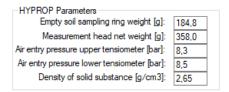


Figure 23 HYPROP Parameters

Table 7 Data Group—HYPROP Parameters

			Editable	by User
Variable	Explanation	Data Value	Public	Power
Empty Soil Sampling Ring Weight	Exact mass of the soil sampling ring (dry and clean).	_	Yes	Yes
	IMPORTANT: This value must be specified individually for each measurement!			
	The mass can be determined before or after the HYPROP 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%.			

# THE REGISTERS—PROCESSING DATA

Table 7 Data Group—HYPROP Parameters (continued)

			Editable	by User
Variable	Explanation	Data Value	Public	Power
Measurement Head Net Weight	Mass of the dry, clean measurement base. The mass includes the two filled tensiometers and the silicon sheet used to separate the head from the 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 contromeasurement. For HYPROP devices that are long in use, METER advises weighing them separately. Wrong values transfer linearly to wrong calculated total water contents. An error of 2.5 g leads to a shif of calculated water contents of 1%.	e ol	No	Yes
	NOTE: DO NOT miss this silicon sheet. Otherwise it leads to an error of approximately to 10 g, which means up to 4% water content.	8		
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 since the 2010 series of METER HYPROP tensiometers. For individual specifications, please follow the detailed instructions given by Schindler et al. (2010b). The air entry points of the ceramic cups change with time and use. Please verify the value from time to time.		No	Yes
Air Entry Pressure Lower Tensiometer	Same as explained above, only 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 data for the soil under investigations are available, this value can be replaced by a measure 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 C.	2.65 g/cm³ d	No	Yes

## SCALE INFORMATION DATA GROUP

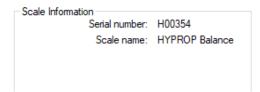


Figure 24 Scale Information

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

Table 8 Data Group—Scale Information

			Editable by User	
Variable	Explanation	Data Value	Public	Power
Serial number	Information given by METER firmware through *.bhdx file.	_	No	No
Scale name	Information as specified in data acquisition software and stored in the *.bhdx file.	_	No	No

## **MEASUREMENT UNCERTAINTY**

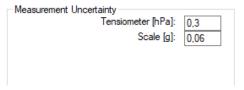


Figure 25 Measurement Uncertainty

# THE REGISTERS—PROCESSING DATA

Table 9 Data Group—Measurement Uncertainty

			Editable by User	
Variable	Explanation	Data Value	Public	Power
Tensiometer	Statistical measurement uncertainty of the tensiometer, i.e., standard deviation of repeated tensiometer readings at a constant physical pressure head. The tensiometer uncertainty is used to eliminate the conductivity values near saturation (Peters, Durner 2008a).	0.3 hPa	No	Yes
	IMPORTANT: The accuracy of the tensiometers is related to random fluctuations (i.e., noise) whereas offsets can lead to systematic errors. Users must control whether the difference of the tensions under hydrostatic conditions is approximately 2.5 hPa. Otherwise erroneous conductivity calculations will occur. In that case, it is advisable to either correct the tensiometer offset (Correction Data Group) or increase the uncertainty of the tensiometers if correcting the tensiometer offset is difficult or impossible.			
Scale	As for the tensiometer. The scale uncertainty eliminates uncertain conductivity data at the end of the measurement campaign, when weight changes between two consecutive time steps become smaller than the scale accuracy.	0.06 g	No	Yes

## **NOTES DATA GROUP**

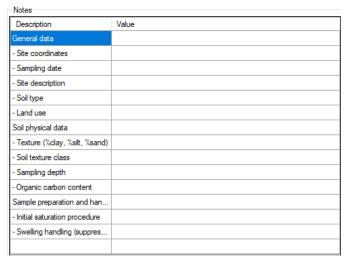


Figure 26 Notes data group

Table 10 Data Group—Notes

			Editable by User	
Variable	Explanation	Data Value	Public	Power
Description	Any information in tabular view.	_	Yes	Yes
	Default value: - General data - Site coordinates - Sampling date - Site description - Soil type - Land use			
	Soil physical data: - Texture (%clay, %silt, %sand) - Soil texture class - Sampling depth - Organic carbon content			
	Sample preparation and handling: - Initial saturation procedure - Swelling handling (suppressed, not suppressed, under load)			
Value	Any information in tabular view.	_	Yes	Yes
Free Data Field	Any informative text can be stored here, that is usefully related to the measurement campaign.	_	Yes	Yes

# 5.2 MEASUREMENTS REGISTER

This section describes how to use the Measurements register for visualization and editing of measured data.

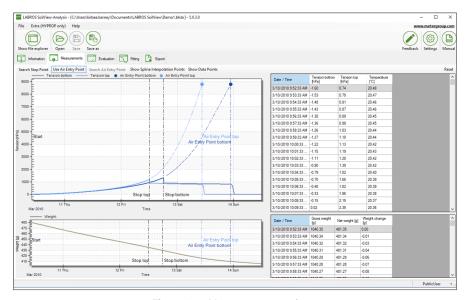


Figure 27 Measurement register

The Measurements register shows the readings of the two tensiometers and the recorded weights. The register is composed of four windows. The two left windows show graphs of the recorded data, and the two right windows show the numerical 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, it 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-mouse button, and selecting the Maximize option in the pop-up menu. Leaving the full-screen mode is reached by pressing the **Esc** key. A user can (repeatedly) magnify portions of the graphs (even in Windows 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 mouse right-button and select the Undo Zoom option.

# 5.2.1 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. Before this cavitation, the water in the tensiometer is due to boiling retardation under a strain, i.e., under negative absolute pressure. When the tension is so high that absolute internal pressure is below

vacuum, the liquid phase at some point suddenly ruptures and a small bubble of vapor arises. This causes the pressure inside the tensiometer to suddenly jump from a negative value to the vapor pressure of water. 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 tension values are 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. The measurement has to be stopped manually by clicking on the respective button. The "end of the data that can be directly evaluated" is automatically detected by the software and indicated by a vertical dashed line by selecting the option "Search Stop Point". The stop line can be manually shifted to an earlier or later time by placing the mouse cursor on the stop line, and dragging it to the left or to the right. The minimum distance between start and stop has to be 2 h. 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, the stop point must occur at a point where the slope of the tension curve is still increasing. Figure 28 illustrates this for the lower tensiometer.

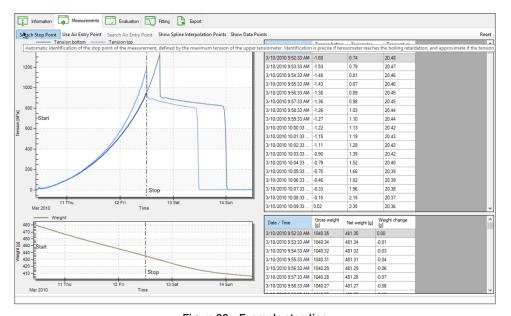


Figure 28 Example stop line

#### THE REGISTERS—PROCESSING DATA

After a certain time with further evaporation, the tensiometer cups will dry out and become permeable to air, meaning that the air entry point of the tensiometer is reached. 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 (= pressure difference between internal water pressure and ambient atmospheric pressure) will go down to zero.

## 5.2.2 DATA VISUALIZATION OPTIONS



Figure 29 Data visualization options

In the header line above the graphs (Figure 29), buttons for data visualization options are listed. They differ for power users and public users. The options are described in Table 11.

Table 11 Data Visualization Option Explanations

	Table 11 Data visualization Option E	Aptanations		
			Editable	by User
Variable	Explanation	Data Value	Public	Power
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. LABROS SoilView-Analysis detects this point automatically by pressing on the Search Stop Point button.	Automatic	Yes	Yes
	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.			
	NOTE: Be aware that the minimum distance between start and full stop has to be 2 hours.			
	If the tensiometer is not filled correctly, the drop might not occur in that sharp manner, since the tensiometer does not reach a cavitation. 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 tensiometer. If the lower tensiometer reaches the point with the highest slope before the upper tensiometer reaches cavitation or falls out, then the stop point has to be set according to the lower tensiometer.			

Table 11 Data Group—Data Visualization Option Explanations (continued)

			Editable by User	
Variable	Explanation	Data Value	Public	Power
Search Stop Point (continued)	If the air entry points are used for evaluation, two stop lines (one for each tensiometer) are shown. Then the stop lines have to be set to the maximum pressure values.	Automatic	Yes	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 5.2.4.	_	No	Yes
Search Air Entry Point	If the Use Air-Entry Point option is activated, and the line that indicates the time of the air-entry point has been moved manually, pressing this button resets to the automatic detection of the air entry time.	Automatic	No	Yes
Show Spline Interpolation Points	Activates and deactivates the depiction of the supporting data points, as described in Section 5.2.3.2.	Automatic	No	Yes
Show Data Points	Activates and deactivates the depiction of the individual measured data points, as described in Section 5.2.3.1.	Automatic	Yes	Yes
Reset	The Reset option resets all settings to default values, in particular the ranges for the visualization of the data in the two graphs.	Automatic	Yes	Yes

#### 5.2.3 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. The unit can be changed between pF, hPa, kPa, MPa and bars by opening the settings window.

#### 5.2.3.1 VISUALIZING MEASURED DATA POINTS

The graph shows the temporal evolution of the tensions as lines without individual dots for the data by default. If desired, a user can additionally visualize 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 (Mark Data Points). When this option is activated, single data points can be easily searched in the data table by clicking on the desired value in the graph. Data points can now be edited or deleted in the table. Deselecting the option, the individual data points disappear again. Data can also be shown by clicking on the respective **ON-OFF** button in the header line above the graph (Show Data Points).

#### THE REGISTERS—PROCESSING DATA

#### 5.2.3.2 VISUALIZING SUPPORTING POINTS USED FOR SMOOTH INTERPOLATION OF DATA

As indicated in Peters and Durner (2008), not all data are used for the calculation of the retention and conductivity data, but just a limited number of support data that are taken from a Hermitian Spline Interpolation of measured data. The actual number of these support data can be selected in the submenu Edit Interpolation Parameters in the Evaluation register (Figure 30). Supporting data can be visualized by clicking on the on-off toggle **Show Spline Support Points** button in the header line directly above the graph.

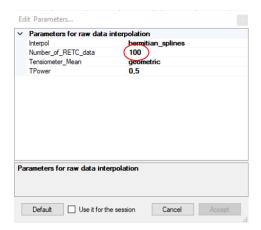


Figure 30 Number of RETC data

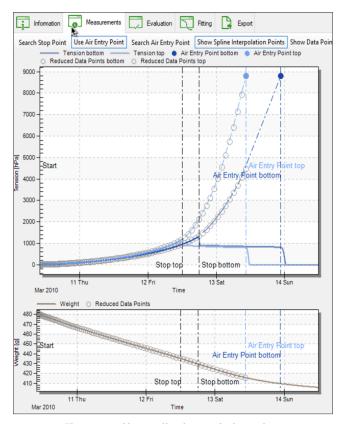


Figure 31 Show spline interpolation points

## 5.2.4 USING THE TENSIOMETER CUP AIR-ENTRY POINT 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 an additional measuring point (Schindler et al., 2010b). The LABROS SoilView-Analysis includes this option for Power Users. The air-entry point is located at the time where the sudden pressure drop of the tensions to zero occurs (Figure 31). 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 (Figure 31) button will add an extra measurement point for each tensiometer that has reached the point where air passes the tensiometer cup. At that point in time a tension that is specified in the Information register > HYPROP Parameters is used to measure tension of the respective tensiometer. The Use Air Entry point button is an on-off switch. Hence, to deactivate the use of the air-entry point, press the button again. At the time axis 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 the **Search Air Entry Point** button.

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 (Figure 31). For the LABROS SoilView-Analysis 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).

Keep in mind that the air entry point of the ceramic cups changes with time and use. Please verify the value from time to time.

#### Gross weight Net weight [g] Weight change Date / Time 480 -470 -3/10/2010 9:52:33 AM 1040.35 481.35 0.00 460 -□ 450 - Start 3/10/2010 9:53:33 AM 1040.34 481.34 -0.01 3/10/2010 9:54:33 AM 1040.32 481.32 -0.03 440 -430 -3/10/2010 9:55:33 AM 1040.31 481 31 -0.04 420 --0.06 3/10/2010 9:56:33 AM 1040.29 481.29 Stop 410 3/10/2010 9:57:33 AM 1040 28 481.28 3/10/2010 9:58:33 AM 1040 27 481 27 -0.08 Mar 2010

## 5.2.5 WEIGHT GRAPH

Figure 32 Weight graph

The lower graph (Figure 27) 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 soil sampling ring, and possibly additional weights, as described in the Information register. 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 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 deactivated 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 potential evaporation rate in the laboratory environment. Small changes in 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 2" 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).

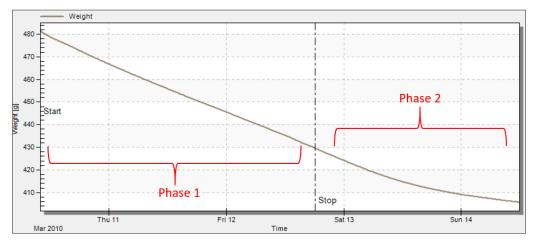


Figure 33 Phases of weight curve

#### 5.2.6 TENSION DATA WINDOW

The window at the upper right (Figure 27) 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 and changes of the contents of individual data cells. Also, multiple lines can be selected, and the data can be copied using the Ctrl+c keyboard combination. Manipulation of data or deletion of data (for power user mode only) will immediately be shown in the graph to the left. By selecting one single measurement point in the graph, the table automatically switches to this measurement line.

#### 5.2.7 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 and changes of the contents of individual data cells. Also, multiple lines can be selected, and the data can be copied with the "ctrl+c" option. Manipulation of data

or deletion of data (for power user mode only) will be immediately shown in the graph to the left. By selecting one single measurement point in the graph, the table automatically switches to this measurement line.

### 5.3 EVALUATION REGISTER

The following section describes how the Evaluations register is used with calculating retention and conductivity data.

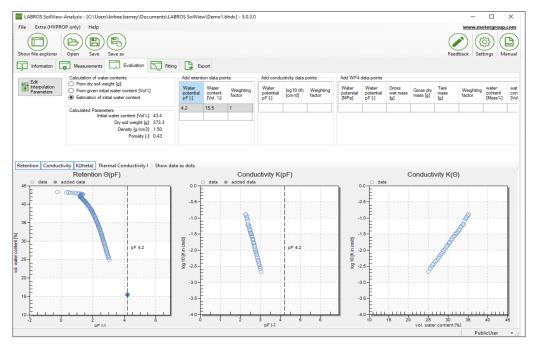


Figure 34 Evaluation register window

The Evaluation register shows five data groups in the upper part with specifications for the calculation of absolute water contents, calculated parameters, and three 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.

By right clicking on one of the graphs, the front size can be changed between small, medium and large and the graph can be maximized. For the first and the second graph there is also the possibility to change between linear or log scaling of the x-axis. Also the units of the x-axis can be chosen between pF, hPa, kPa, MPa and bars.

#### 5.3.1 RETENTION AND CONDUCTIVITY DATA CALCULATION

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. (2010 a,b), Peters and Durner (2008) and Peters et al. (2015). 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 Section 5.2, are considered.

#### 5.3.2 ABSOLUTE WATER CONTENTS CALCULATION

The relative shape 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.

#### OPTION 1: INITIAL WATER CONTENT CALCULATION FROM DRY SOIL WEIGHT

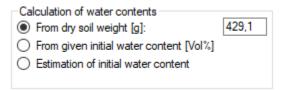


Figure 35 Water content calculation

This is the option of choice if the dry soil weight has been determined after the end of the measurement, by oven-drying at 105 °C for 24 h. The exactness of the result depends on the correctness of all involved parameters that are specified in the Information register. From the data, further soil physical parameters such as the initial water content, the porosity and the dry bulk density are also calculated and shown in the underlying group Calculated Parameters.

NOTE: Only option 1 leads to a 100 % correct calculation of the absolute water content.

#### OPTION 2: USER-SET INITIAL WATER CONTENT EXTERNAL SETTING

Calculation of water contents	
From dry soil weight [g]:	
● From given initial water content [Vol%]	36,0
Estimation of initial water content	

Figure 36 User-set water content calculation

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: INITIAL WATER CONTENT AUTOMATIC ESTIMATION**

Calculation of water contents
From dry soil weight [g]:
From given initial water content [Vol%]
Estimation of initial water content

Figure 37 Initial water content estimation

If the dry weight of the soil is not yet available, the initial water content of the measurement 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. As a result of the assumptions, the initial water content, the porosity, the 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 provided in Appendix B.

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. Be aware that the calculation is always based on the chosen option.

IMPORTANT: The calculation of porosity and absolute water content 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/cm³), mass of the measuring head, mass of the sampling ring that contains the sample, and mass of dry soil which is specified in the Evaluation register. Any error in these data will be linearly transferred to the results. Furthermore, overfilling or underfilling of the sampling rings with soil will cause appreciable errors. As a rule of thumb, 1-mm error in sample height causes about 2% error in the calculated data.

## 5.3.3 ADDING INDEPENDENT RETENTION AND CONDUCTIVITY DATA

Add retention data points Add conductivity data points				Add WP4 data points									
Water potential pF [-]	Water content [Vol. %]	Weighting factor	Water potential pF [-]	log10 (K) [cm/d]	Weighting factor	Water potential [MPa]	Water potential pF [-]	Gross wet mass [g]	Gross dry mass [g]	Tare mass [g]	Weighting factor	water content [Mass%]	water content [Vol%]
4,67	11,37	1	-3	2,06	1	1,9055	4,28	29,006	28,238	24,955	1	23,39	40,24
5,05	8,76	1			1						1		

Figure 38 Add independent retention and conductivity data

Users can add independently measured data from the METER WP4C or pressure plate measurements as well as conductivity measurements taken with the METER KSAT®.

If the respective volumetric water content for the additional water potential point is already calculated, the values can be added in the first table. Entering water potential, gross wet mass, gross dry mass and tare mass in the third table, LABROS SoilView-Analysis automatically calculates the water content.

The entered data points are displayed as filled dots in the graphs below, whereas the HYPROP-measured data are shown as empty circles.

Please care for the appropriate units when adding the data: tensions must be added in the displayed units which can be changed in the settings, conductivity data has to be added as a 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:

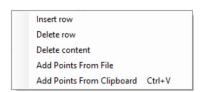


Figure 39 Edit independent retention and conductivity data

As an additional feature, retention and/or conductivity points can be read from Excel data files (.xlsx) or inserted with using copy and paste instead of entering manually. This is of particular advantage if many points are available from independent measurements.

By using copy and paste, please be sure to keep the right numbers of fields (maximum of three fields for the Add retention data points table and the Add conductivity data points; maximum of six fields for the Add WP4 data points table) and the correct sequence. Also please care for the regional conventions for the decimal separator (comma or dot), as specified in the Windows System Software. The insertion starts in the current active field.

By using the Add points from file option, please be sure to keep the right numbers of fields (maximum of two fields for the Add retention data points field and the Add conductivity data points; maximum of four fields for the Add WP4 data points table) and the correct sequence. Also please care for the regional conventions for the decimal separator (comma or dot), as specified in the Windows System Software. In addition it is necessary to have the same heading as the columns of the tables. The insertion starts in the first new line.

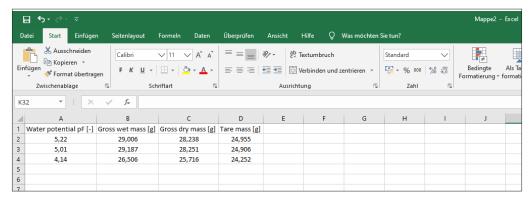


Figure 40 Adding WP4 data points file format

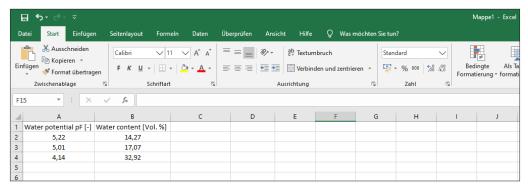


Figure 41 Adding retention data points file format

## **5.3.4 MODIFYING EVALUATION PARAMETERS**

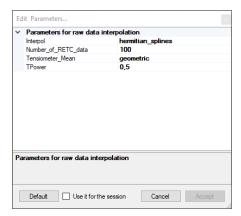


Figure 42 Edit interpolation parameters

The parameters for raw data interpolation can be edited in a submenu, which pops up when clicking on the respective **Edit Interpolation Parameters** button on the right side of the header line in Evaluation register. The interpolation parameters are described in Table 12.

Table 12 Interpolation parameters

			Editable	by User
Variable	Explanation	Data Value	Public	Power
Interpol	Determines the interpolation mode for the measured data:	2	Yes	Yes
	1: piecewise_linear 2: hermitian_splines			
Number_of_RETC_data	Number of support points for hydraulic functions (<1000). Note that this number is valid for the resulting retention data. Internally the same number of conductivity data is calculated but the invalid data near saturation are not shown.	100	Yes	Yes

Table 12 Interpolation parameters (continued)

			Editable	by User
Variable	Explanation	Data Value	Public	Power
Tensiometer_Mean	Determines the calculation mode for the mean tension for the calculation of the water retention curve points:	3	Yes	Yes
	1: arithmetic 2: geometric 3: mixed (see Peters et al. 2015)			
TPower	Determines the spacing of the support points for the spline interpolation. A value 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.	0.5	Yes	Yes

#### 5.3.5 SETTING WINDOW

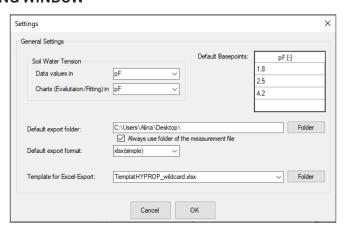


Figure 43 Setting window

By selecting the settings button in the upper right corner a setting window appears. Here the user can select the unit for the data values as well as for the charts. Furthermore base points can be added and customized. Also export folder and format can be selected. By ticking the box, the export files will be saved in the same folder as the measurement file. It is also possible to customize the export template. The default template is saved on the local drive in the same folder as the software. This template can be copied and edited. The user can delete, add or change information (except the fields in brackets as these are filled automatically).

By clicking the **OK** button, these settings are set as default for all further measurements.

## 5.4 FITTING REGISTER

This section describes how the Fitting register fits hydraulic functions to the data.



Figure 44 Fitting register

For use in numerical modeling, hydraulic characteristics are described by parametric functions for  $\theta(h)$  and K(h), or  $K(\theta)$ , where  $\theta$  is the volumetric water content, K the hydraulic conductivity and h the matric potential. LABROS SoilView-Analysis provides a high-class algorithm to fit a wide variety of functional relationships of the retention curve and the conductivity curve to the data. No specification of initial guesses for the parameter values is required.

Sixteen widely-used retention models are available, encompassing the expressions of Brooks and Corey, Fredlund-Xing, Kosugi and van Genuchten with and without parameter constraint for the parameter m. With the exception of Brooks-Corey model, all functions are available as PDI-variant in uni- and bimodal form. The PDI-variant ensures that the water content matches zero at oven dryness, and it considers the effect of water in capillaries, in films and in corners of pores, in both the retention function and conductivity function. All models are described in Appendix C.

#### 5.4.1 FITTING FUNCTIONS

The Fitting register contains a header line with the fit button (Curve Fitting) and the option of editing "Optimization Parameters" at left, and a button for "Restore Parameters" at 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 section 5.4.6). The "Restore Parameters" button will reset all values for the parameter bounds to the default values.

To fit the selected hydraulic functions to the data, click on the **Curve Fitting** button. A window will pop up (Figure 45) that indicates that the fitting routine is running. This process can last as long as a few seconds or as long as 1 or 2 min, depending on the selected model and the number of data points. It cannot be stopped or otherwise interrupted.

NOTE: In cases where the fitting will apparently not lead to a stop, the user can cancel the process in the Windows Task Manager.

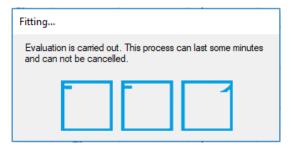


Figure 45 Fitting process window

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 multiobjective 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 (Section 5.4.6).

#### 5.4.2 SELECTING A MODEL AND SPECIFYING PARAMETER BOUNDS

A hydraulic model is selected by marking the respective tick box. By default, all model parameters are included in the fitting process (except the parameters `pF\_dry` and `a` for the PDI models), 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 bandwidth, by changing the default minimum and maximum value, but for most soils, this will not be necessary. In other cases, users may have prior knowledge about parameters that can lead to much reduced bandwidths, which speeds up the convergence of the algorithm.

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 "Retention function parameters" and "Conductivity function parameters". 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. Default values can be re-entered by selecting "Restore Parameters".

If the tick-box in front of the parameter is selected, the value will be calculated automatically. By deselecting the tick-box, the default value is shown and the value can be entered manually. If a model selection is changed, the user is asked if he wants to keep the manual changed values for the fitting parameter or not.

NOTE: For the decimal separator (i.e., appropriate use of comma or dot in the inserted numbers), the regional conventions of the Windows system are used.

#### 5.4.3 PARAMETER ESTIMATION AND UNCERTAINTY MEASURES RESULTS

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 following two columns). The mathematical background for the calculations of uncertainties is given in Appendix C (SHYPFIT2.0). 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. Fit quality is given in terms of the root mean square errors, separately calculated for the water content data (RMSE\_TH) and the log of conductivities (RMSE\_K). The root mean squared error 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. 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.

As an aid in deciding which model is most appropriate, LABROS SoilView-Analysis additionally shows the corrected Akaike Information Criterion (AICc, Akaike, 1974; Hurvich, Tsai, 1989) in the field. This criterion accounts for the different number of adjustable parameters when selecting the best model. The value will normally be negative. The smaller the value (i.e., the larger the absolute number), the more appropriate is the model. Note that the actual value of the AICc has no meaning. It can only be used to compare different model fits for one set of data. For details on the statistical criteria, see Appendix C (SHYPFIT).

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 selecting the respective option in the Optimization Parameters menu (Section 5.4.6).

As indicated above, models with a higher number of parameters are generally more flexible. But will have 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 I	Matrix										
	alpha1	n1	th_r	th_s	alpha2	n2	w2	Ks	tau	omega	^
▶ alpha1	1,000	0,830	0,893	-0,315	-0,645	0,095	0,145	-0,191	0,191	0,906	
n1	0,830	1,000	0,990	-0,664	-0,881	0,058	0,106	-0,145	0,144	0,986	
th_r	0,893	0.990	1,000	-0,620	-0,854	0,072	0,122	-0,163	0,163	0,996	
th_s	-0,315	-0,664	-0,620	1,000	0,652	-0,010	-0,032	0,048	-0,048	-0,604	
alpha2	-0,645	-0,881	-0,854	0,652	1,000	-0,397	-0.447	0,493	-0,493	-0,843	
n2	0,095	0.058	0,072	-0,010	-0,397	1,000	0,997	-0,977	0,977	0,068	
w2	0,145	0,106	0,122	-0.032	-0.447	0,997	1,000	-0,990	0,990	0,118	
Ks	-0,191	-0,145	-0,163	0,048	0,493	-0,977	-0.990	1,000	-1,000	-0,160	
tau	0,191	0,144	0,163	-0,048	-0,493	0,977	0,990	-1,000	1,000	0,160	_
<										2	>

Figure 46 Correlation matrix

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 overparameterization of the selected model.

#### 5.4.4 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 95% confidence intervals are shown here as grey shaded areas if selected before. 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 LABROS SoilView-Analysis 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 Export register (Section 5.5).

#### 5.4.5 FIELD CAPACITY AND PLANT AVAILABLE WATER

```
Field capacity

WC @ 6 kPa 26,7 %

WC @ 33 kPa 21,4 %

WC @ 1500 kPa 8,1 %

PAW 6_1500 kPa 18,6 %

PAW 33...1500 kPa 13,3 %
```

Figure 47 Field capacity

Retention curves are often determined to get estimates of field capacity and plant available water. LABROS SoilView-Analysis shows the corresponding values immediately after each fit. The calculation is based on the fitted curves and encompasses:

WC@6 kPa = water content at pF 1.8 (i.e., field capacity for conditions with close groundwater level)

WC@33 kPa = water content at pF 2.5 (i.e., field capacity for conditions distant to groundwater)

WC@1500 kPa = water content at pF 4.2 (i.e., at the wilting point)

PAW 6 ... 1500 kPa = plant available water as difference of water contents at 6 and at 1500 kPa

PAW 6 ... 1500 kPa = plant available water as difference of water content at 33 and at 1500 kPa

### 5.4.6 MODIFYING OPTIMIZATION PARAMETERS

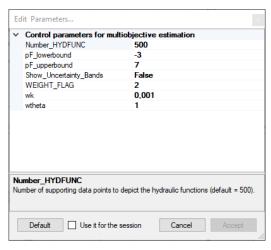


Figure 48 Edit fitting parameters

Users can edit some of the parameters that specify the calculations and the depiction of the fitted functions. The specifications are listed by selecting the button Optimization Parameters and described in Table 13.

Table 13 Optimization Parameters

			Editable	by User
Variable	Explanation	Data Value	Public	Power
Number_HYDFUNC	The hydraulic functions in the graphs are taken from internal tables, where the functions are listed in the range PFBOUNDS_LOWER to PFBOUNDS_UPPER at discrete supporting points. Number_HYDFUNC is the number of supporting data points to depict the hydraulic functions.	500	Yes	Yes
	NOTE: This also affects the number of data written in the exported tables.			
pF_lowerbound	Lower bound for internal table of hydraulic functions, expressed as pF (=log10(h) with h in cm). The default value expresses a minimum tension of 0.001 cm.	-3	Yes	Yes
pF_upperbound	Upper bound for internal table of hydraulic functions, expressed as pF (=log10(h) with h in cm). The default value is pF = 7, which is a tension of 10,000,000 cm.	7	Yes	Yes
Show_Uncertainty_Bands	Flag for showing the 95% uncertainty bands for the fitted functions in the depicted graphs by a grey shading.	False	Yes	Yes

Table 13 Optimization Parameters (continued)

			Editable	by User
Variable	Explanation	Data Value	Public	Power
WEIGHT_FLAG	The simultaneous fit hydraulic functions to retention data and conductivity data is a multiobjective minimization problem, which requires weights for the data of the different data types. LABROS SoilView-Analysis provides the possibility to either prescribe these weights, 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. 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 103.	2	Yes	Yes
	O: weights for data classes as specified by user (parameters wk and wtheta), internal weights in each class are scaled by distance to neighbouring data points			
	1: as 0, but weights for data classes are calculated automatically as described by Peters and Durner (2008)			
	2: as 0, but data of same type have all the same weight (= default)			
wk	Weight of the conductivity data class. Default = 0.001	0.001	Yes	Yes
wtheta	Weight of the retention data class. Default = 1.0	1.0	Yes	Yes

## 5.5 EXPORT REGISTER

This section describes how the Export register supports exporting data, graphs, functions and parameters.

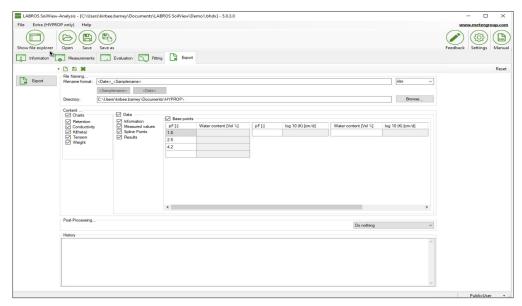


Figure 49 Export register

The Export register allows the export of all graphs, raw data, calculated data, fitted functions, and other parameters of interest. User specifications for data format, file name convention and directory will be kept as default as long as the user remains in this session.

LABROS SoilView-Analysis supports the following output file formats (Table 14):

Table 14 Output File Formats

	·
Variable	Explanation
xlsx	Microsoft Excel file format. The Excel file will contain all relevant data in different sheets:  • Configuration and information  • Measured raw data  • Data from spline interpolation used to derive retention and conductivity data  • Retention and conductivity data  • Data of fitted curves  • Parameters of fitted models  • Fitted model parameter uncertainties  • Base points (if specified)
xlsx (simple)	Microsoft Excel file format for import (File >Import menu) into LABROS SoilView-Analysis software.  The Excel file will contain one sheet with parameters and one sheet with the measurement data (tension and weight).

Table 14 Output File Formats (continued)

Variable	Explanation
HYDRUS table	File named MATER.IN, readily formatted for direct use in HYDRUS simulations. The file contains retention curve, specific water capacity, and conductivity data.
CSV	Comma-separated values, for editing with any external program.
csv (simple)	Comma-separated values for re-import into LABROS SoilView-Analysis software. Creates three files <name>_Config.csv, <name>_Tension.csv, <name>_Weight.csv, which contain the respective data. These files can be manipulated outside of HYPROP and imported using the File &gt;Import menu.</name></name></name>

#### 5.5.1 OUTPUT SETTINGS

Different output settings are available and described below. To export, left-click on the **Export** button.

#### **FILE NAMING**



Figure 50 File name

Enter the output file name in the field Filename format. All permitted characters can be used in the file name. The two default settings <Date> and <Sample name> are available for optional use in any position within the file name. They will automatically be replaced by the current date or sample name.

#### **FILE FORMAT**

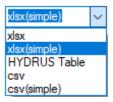


Figure 51 File format

Select different file formats in the pull down menu.

#### DIRECTORY



Figure 52 File name

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

#### **5.5.2 CONTENT**

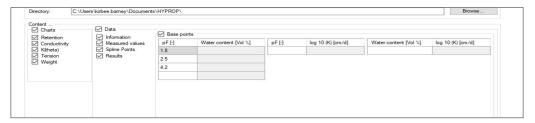


Figure 53 Edit fitting parameters

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

In the Diagrams group, select the checkboxes for the diagrams that should be exported.

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

These functions are only available for export formats .xlsx and .csv.

It is possible to enter freely definable base points for which the correlating data points will be calculated. To do so, enter the desired value in the table, and correlating data points are automatically calculated and exported when exporting is executed. Left-click the **Update** button to update the data points.

#### 5.5.3 POST-PROCESSING

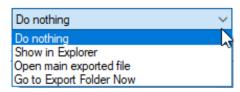


Figure 54 Post-processing

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

## 5.5.4 HISTORY



Figure 55 History

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

## Measurements Evaluation Fitting Export 1 476 1.288 1 786 0.937 0.043 1.832 pF\_dr 2.052 Model: VGbi-PDI Model Code: 1211 ource: Iden and Dumer (2014), Peters (2014) escription: PDI-variant of the bimodal constrain Retention | Conductivity | K(theta) | Thermal Conductivity | | Show data as dots Retention Θ(pF) Conductivity K(pF) Conductivity K(Θ)

## 6. PROCESSING MULTIPLE DATA SETS

Figure 56 Multiple data sets

LABROS SoilView-Analysis 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 \*.bhdix). 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 \*.bhdx files to a \*.bhdix project is described in the Extras command menu, Section 4.2.3. Once individual measurement campaigns are combined, they can be activated and deactivated simply by clicking on the individual tick boxes in the file explorer.

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 \*.bhdix file contains copies of the original data). Clicking on the \*.bhdix name will return to the combined project menu (Figure 56).

## 7. SERVICE

This section provides customer service information.

## 7.1 CUSTOMER SUPPORT

#### NORTH AMERICA

Customer service representatives are available for questions, problems, or feedback Monday through Friday, 7:00 am to 5:00 pm Pacific time.

Email: support.environment@metergroup.com

sales.environment@metergroup.com

Phone: +1.509.332.5600

Fax: +1.509.332.5158

Website: metergroup.com

#### **EUROPE**

Customer service representatives are available for questions, problems, or feedback Monday through Friday, 8:00 to 17:00 Central European time.

Email: support.europe@metergroup.com

sales.europe@metergroup.com

**Phone:** +49 89 12 66 52 0 **Fax:** +49 89 12 66 52 20

Website: metergroup.de

If contacting METER by email, please include the following information:

Name Email address

Address Instrument serial number

Phone Description of the problem

NOTE: For products purchased through a distributor, please contact the distributor directly for assistance.

## 7.2 TERMS AND CONDITIONS

By using METER instruments and documentation, you agree to abide by the METER Group. Terms and Conditions. Please refer to metergroup.com/terms-conditions for details.

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## APPENDIX A. EVAPORATION METHOD THEORY

This appendix describes the theory behind the HYPROP.

In a soil sampling ring two tensiometers are installed at two depths ( $z_1$  and  $z_2$ ). The middle height between the sensing tips of the tensiometers is the central plane 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 the atmosphere so that the soil water can evaporate. From the soil water tension [hPa] 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 flow rate.

A measuring campaign will last until one of the tensiometers runs dry, the mass changes become marginal, or, if the air entry values of the tensiometers is used, until both tensiometers reach the air entry value. Then, the dry weight of the soil is determined by oven drying the sample at 105 °C for 24 h. With these values the retention curve and the unsaturated conductivity is calculated as described next.

First, an interpolation scheme is applied to the raw data for the measured time series of tensions and weights to get N interpolated data for each data series at the same times,  $t_p$ . The user can choose between linear interpolation and Hermitian spline interpolation. As default, the LABROS SoilView-Analysis software uses Hermitian spline interpolation and N = 100.

The total mass of water  $\omega_i$ , at time  $t_i$  is derived from the weight measurements at time  $t_i$  by subtracting the weights of the tare components from the total weight  $\omega_{tot}(i)$  recorded by the LABROS balance at times  $t_i$ . The tare weights in a standard HYPROP measurement campaign are the weight of the empty steel cylinder  $\omega_{cyl}$ , the weight of the HYPROP base including the tensiometer shafts and the silicon mat  $w_{HYP}$ , and the weight of the dry soil  $\omega_{soil}$ . Thus,  $\omega_i = \omega_{tot}(i) - \omega_{cyl} - \omega_{HYP} - \omega_{soil}$ . Dividing  $\omega_i$  by the density of water, which is assumed to be equal to 1 g/cm<sup>-3</sup>, gives the water volume  $V_w$  [cm<sup>3</sup>]. The mean water content of the column,  $\theta i$  [–] at time  $t_i$  is computed by dividing the volume of water by the column volume V.

To obtain water retention data pairs, the mean water contents at time

$$t_{_{i-1/2}} = \frac{1}{2} \big( t_{_{i-1}} + t_{_i} \big) \label{eq:time_time_time}$$
 Equation 1

Equation 2

are calculated by

$$\overline{\theta}_{i-1/2} = \frac{\theta_i + \theta_{i-1}}{2}$$

In the original data evaluation (Peters and Durner, 2008, Schindler et al., 2010), the arithmetic mean of the four measured suctions, h [cm] is used as shown in Equation 3,

$$\overline{h}_{ari,i-1/2} = \frac{h_{1,i} + h_{1,i-1} + h_{2,i} + h_{2,i-1}}{4}$$
 Equation 3

#### **EVAPORATION METHOD THEORY**

where subscripts 1 and 2 represent the location of the tensiometers (i.e., 1 is lower and 2 is upper tensiometer). However, Peters et al. (2015) showed that only in the beginning of the measurement, when the suction distribution is close to the hydrostatic conditions, the arithmetic mean of the suctions is preferable. In later stages, the suction distribution becomes highly nonlinear. Then the geometric mean for the two tensiometers is preferable (Equation 4):

$$\overline{h}_{geo,i-1/2} = \frac{\sqrt{\left(h_{1,i} + h_{1,i-1}\right) + \left(h_{2,i} + h_{2,i-1}\right)}}{2}$$
 Equation 4

To get the most appropriate mean suction at any time, Peters et al. introduced the mixed mean, which is given by Equation 5:

$$\overline{h}_{\text{mix},i-1/2} = \omega_{\text{avg}} \overline{h}_{\text{ari},i-1/2} + \left(1 - \omega_{\text{avg}}\right) \overline{h}_{\text{geo},i-1/2}$$
 Equation 5

where  $w_{avg}$  [–] is a weighting parameter that controls the shift from the arithmetic to the geometric mean. As a weighing parameter, LABROS SoilView-Analysis simply uses the inverse to the SEM-approximated gradient in suction  $\nabla h$  (Equation 6):

$$\omega_{\text{avg}} = \frac{1}{\nabla h}$$
 Equation 6

For conditions close to hydrostatic conditions, where the approximated gradient of the suction  $\nabla h$ : is close to unity,  $\overline{h}_{_{\text{mix},l-1/2}}$  is close to the arithmetic mean, whereas in later\_stages of the experiments, when the suction distribution in the column is highly nonlinear,  $h_{_{\text{mix},l-1/2}}$  is close to the geometric mean. The LABROS SoilView-Analysis calculates the retention data always between two interpolated times and not for the interpolated time steps. This is done to get exact data triplets for water contents, suctions, and conductivities. The calculation of conductivity data relies on flux data and thus, requires the data at two different time steps (Equation 7).

For the calculation of unsaturated hydraulic conductivity,  $K[cm\ d^{-l}]$ , first estimate the water flux at the column center,  $\hat{q}_c[cm\ d^{-l}]$ . For any time  $t_{i^-1/2}=1/2(t_{i^-1}+t_{i^-})\hat{q}_c$  is assumed to be half of the evaporation rate  $q_o[cm\ d^{-l}]$  (Equation 7):

$$\hat{q}_{c,i-1/2} = \frac{q_{0,i-1/2}}{2} = \frac{L}{2l} \frac{L\bar{\theta}_i - \bar{\theta}_{i-1}}{\Delta t_{i-1/2}}$$
 Equation 7

where  $\Delta t_{i-1/2} = t_i - t_{i-1}$  and *i* runs from 2 to N, the number of data points. The mean gradient of the hydraulic head at the center of the column is then approximated as shown in Equation 8:

$$\nabla H_{i-1/2} = \frac{\bar{h}_{1,i-1/2} - \bar{h}_{2,i-1/2}}{z_2 - z_1} - 1$$

**Equation 8** 

where  $\overline{h}_{I,i-I/2}$  and  $\overline{h}_{2,i-I/2}$  are the mean suctions at the two depths  $z_I$  [cm] and  $z_2$  [cm] in the time interval  $\Delta t_{i-I/2}$  which are calculated by the arithmetic mean in time. The hydraulic conductivity K [cm  $d^{-I}$ ] is then calculated according to the Darcy-Buckingham law as shown in Equation 9:

$$K_{\scriptscriptstyle i-1/2} = \frac{\hat{q}_{\scriptscriptstyle c,i-1/2}}{\nabla H_{\scriptscriptstyle i-1/2}} \label{eq:Kindowski}$$
 Equation 9

These conductivity data are assigned to mean suctions  $\overline{h}$  to obtain data for K(h). Thus, at each time  $t_{i-1/2}$  a triplet of data points for  $\overline{h}, \overline{\theta}$  and K is obtained leading to a full set of  $\theta(h)$ , K(h),  $K(\theta)$ .

As previously described, LABROS SoilView-Analysis offers three approaches to calculate the mean suction

h, the arithmetic, geometric, and mixed mean. It is strongly recommended to use the mixed mean, which is also the default.

A limitation of the evaporation method is that at the beginning of the experiment, the hydraulic conductivities are usually much higher than the fluxes, and the gradients of the hydraulic head  $\nabla H$  are therefore small. Because of inevitable noise of tensiometer measurements reflecting measurement and calibration error, very small gradients cannot be resolved and hydraulic conductivities, which are much higher than the flux q, cannot be determined with sufficient accuracy. To account for this, the criterion used by Peters and Durner (2008) is applied to reject all data that are calculated from gradients smaller than  $6\sigma_b/\Delta z$ , where  $\sigma h$  is the measurement noise of the tensiometer readings.

NOTE: In LABROS SoilView-Analysis 5.0 the default value for the tensiometer uncertainty is set to  $\sigma h = 0.15$  hPa. This means that even small systematic offset shifts in tensiometer readings can easily lead to erroneous results and must be strictly avoided. If set properly, suctiony must differ in the initial phase of an evaporation experiment, when almost hydrostatic conditions prevail, by exactly 2.5 cm.

# APPENDIX B. INITIAL WATER CONTENT AUTOMATIC ESTIMATION

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 drying for 24 h at 105 °C. If this value is not yet available, a guess of the initial water content can be obtained using the LABROS SoilView-Analysis software using Equation 10,

$$\theta_{s} = 1 - \frac{m_{0} - \rho_{w} \times V_{tot}}{\left(\rho_{s} - \rho_{w}\right) \times V_{tot}}$$

Equation 10

where

 $\theta_s$  (cm³ cm⁻³) is the saturated volumetric water content, equal to the porosity and assumed to be the initial water content

 $p_{w}$  (g cm<sup>-3</sup>) is the density of water, taken to be 1.0 g cm<sup>-3</sup>

 $p_s$  (g cm<sup>-3</sup>) is the density of the soil matrix

 $V_{tot}$  (cm<sup>3</sup>) is the volume of the soil sample

 $m_0$  (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 specified in the Information register.

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 Evaluation register.

## APPENDIX C. SHYPFIT2.0 USER'S MANUAL

Authors: Andre Peters and Wolfgang Durner, 2015

Cite as: Peters, A. and Durner, W. (2015). SHYPFIT 2.0 User's Manual. Research Report. Institut für Ökologie, Technische Universität Berlin, Germany.

LABROS SoilView-Analysis uses SHYPFIT2.0 for selecting and fitting different soil hydraulic models to the data. The model structure in SHYPFIT2.0 follows the PDI model suggestion, which combines water retention and conductivity in completely and incompletely filled capillaries as well as isothermal vapor conductivity (Peters, 2013; Iden and Durner, 2014; Peters, 2014). The commonly used retention models of van Genuchten (1980), Kosugi (1996) or the bimodal model of Durner (1994) in combination with the Mualem (1976) hydraulic conductivity model are given as special cases of the general PDI models as will be outlined below.

## C.1 PDI MODEL COMBINATIONS

This section describes PDI model combinations.

#### C.1.1 RETENTION FUNCTIONS

This section describes retention functions.

#### C.1.1.1 GENERAL

The general form of the PDI retention model is given by the sum of capillary and adsorptive water retention (Peters, 2013; Iden and Durner, 2014):

$$\theta(h) = (\theta_s - \theta_r)S^{cap} + \theta_r S^{ad}$$

Equation 11

Where

 $\theta$  [-] is the volumetric water content

h [cm] is the suction

 $S^{cap}$  [-] and  $S^{ad}$  [-] are the saturation of capillary and adsorptive water retention

 $\theta_{s}$  [-] is saturated water content

 $\theta_{r}$  [-] is the maximum water content for water adsorption

Capillary retention  $\theta^{cap}(h)$  is given by the first term on the right side of Equation 11 and adsorptive retention  $\theta^{ad}(h)$  by second term. Setting  $S^{ad}$  to 1 gives the original capillary retention functions with residual water content. A typical unimodal PDI soil water retention function is shown in Figure 57.

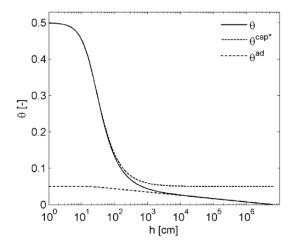


Figure 57 Typical unimodal PDI soil water retention function. The capillary part is here expressed as  $\theta^{\text{cap}*} = \theta^{\text{cap}} + \theta^{\text{r}}$ . Thus  $\theta^{\text{cap}*}$  resembles the classic soil water retention function with residual water content.

#### C.1.1.2 ADSORPTIVE SATURATION FUNCTION

The saturation function for water adsorption is given by a smoothed piecewise linear function (Iden and Durner, 2014):

$$S^{ad}(x) = 1 + \frac{1}{x_a - x_b} \left\{ x - x_a + b \ln \left[ 1 + exp \left( \frac{x_a - x}{b} \right) \right] \right\}$$
 Equation 12

Where  $x = pF = \log_{10} (h \text{ in cm})$ ,  $x_a = \log_{10} (h_a)$  and  $x_0 = \log_{10} (h_0)$  with  $h_a$  being the suction at air entry for the adsorptive retention and  $h_0$  being the suction, where the water content is 0. The parameter  $h_a$  is given as 1/alpha for the unimodal van Genuchten saturation functions and set to  $h_a$  for the basic Kosugi function. For the bimodal functions,  $h_a$  is derived from the highest value of alpha and the lowest value for  $h_a$ , corresponding to the coarsest subfunctions. The parameter h might be set to  $10^{6.8}$  cm, which is the suction at oven dryness for 105 °C (Schneider and Gnoss, 2012). The smoothing parameter h is dependent on the capillary saturation function h000 set h101 set h102 set h103 set h104 set h105 set h105 set h106 set h106 set h107 set h108 set h109 set h

#### C.1.1.3 CAPILLARY SATURATION FUNCTION

The formulation of the saturation function for capillary saturation,  $S^{cap}$  must ensure that the water content is 0 at  $h = h_0$ . This is guaranteed by scaling the basic classic saturation functions,  $\Gamma$  (h) (e.g., van Genuchten, 1980, Kosugi, 1996):

$$S^{cap}(h) = \frac{\Gamma(h) - \Gamma_0}{1 - \Gamma_0}$$

**Equation 13** 

Where  $\Gamma_0$  is the basic function at  $h=h_0$ . Setting  $\Gamma_0=0$  yields the original capillary saturation functions where:

$$S^{cap}(h) = \Gamma(h)$$
 Equation 14

Thus, SHYPFIT2.0 distinguishes between scaled (Equation 13) and unscaled (Equation 14) capillary retention. The effect of scaling according to Equation 13 is exemplarily shown for the van Genuchten function in Figure 58. For small values for n (i.e., wide pore size distributions) the saturation of unscaled function does not reach a value of 0 at oven dryness at  $h = h_0$ .

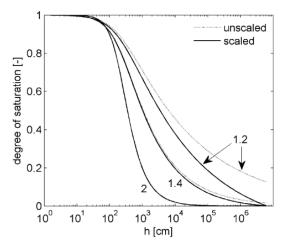


Figure 58 Effect of scaling the capillary retention function according to Equation 13 using the van Genuchten function as basic function. Unscaled is the original  $S^{cap}(h) = G(h)$  function and scaled means  $S^{cap}(h) = (\Gamma(h) - \Gamma_0)/(1 - \Gamma_0)$ . Numbers indicate different values for n.

The basic functions implemented in SHYPFIT2.0 are the constrained and unconstrained unimodal function of van Genuchten (1980), the unimodal function of Kosugi (1996) and part of the original Fredlund and Xing (1994) function. Each of the functions is also given in the bimodal form (e.g., Durner, 1994 for the van Genuchten function and Romano et al., 2011 for the Kosugi function). The constrained function of van Genuchten (1980) is given by Equation 15:

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

Equation 15

Where  $\alpha[1/cm]$  and n [-] are curve shape parameters. The unconstrained function of van Genuchten (1980) is given by Equation 16:

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

**Equation 16** 

Where m [–] is an additionally shaped parameter. The unimodal Kosugi retention function is given by Equation 17:

$$\Gamma(h) = \frac{1}{2} \operatorname{erfc} \left[ \frac{\ln \left( \frac{h}{h_m} \right)}{\sqrt{2}\sigma} \right]^m$$

**Equation 17** 

Where  $h\_m$  is the suction corresponding to the median pore radius,  $\sigma$  [–] is the standard deviation of the log-transformed, pore-size distribution density function and erfc [–] denotes the complementary error function. The basic Fredlund and Xing function is given by Equation 18:

$$\Gamma(h) = \left[ \frac{1}{In\{e + (\alpha h)\}} \right]^{m}$$

Equation 18

**Equation 19** 

where  $\infty$  [1/cm] n [–] and m [–] are curve shape parameters and e [–] is the Euler number ( $e \approx 2.718$ ).

The bimodal functions are weighted sums of the unimodal functions Equation 19:

$$\Gamma(h) = \sum_{i=1}^{2} w_i \Gamma_i$$

Where  $\Gamma_i$  are the weighted subfunctions of the system, expressed by one of the unimodal functions and  $w_i$  [–] are the weighting factors for the subfunctions, subject to  $0 < w_i < 1$  and  $\Sigma w_i = 1$ . Thus three basic functions, which are either uni– or bimodal are implemented. These functions can be scaled according to Equation 13 or not scaled. Furthermore, the adsorption function might be added or not (in that case  $S^{ad}$  in Equation 11 is simply set to 1). All in all this gives 24 combinations for the soil water retention function (basic functions: 3; modality: 2; scal: 2; ads: 2) are possible (see Table 15). The unscaled unimodal van Genuchten function without adsorption (first line in Table 15) is the original van Genuchten function. The shape parameter b for the adsorption function (Equation 11) is given by Equation 20:

$$b = 0.1 + \frac{0.2}{n^2} \left\{ 1 - exp \left( -\frac{\theta_r}{\theta_s - \theta_r} \right)^2 \right\}$$

**Equation 20** 

for the constrained and unconstrained van Genuchten and Fredlund and Xing functions and by Equation 21:

$$b = 0.1 + 0.07\sigma \left\{ 1 - exp \left( -\frac{\theta_r}{\theta_s - \theta_r} \right)^2 \right\}$$

Equation 21

for the Kosugi function. For the bimodal functions, n and  $\sigma$  are taken from the coarsest subfunction (i.e., the subfunction with highest value for  $\alpha$  or the lowest value for  $h_m$ ).

Figure 59 shows a bimodal scaled water retention function with capillary and adsorptive part.

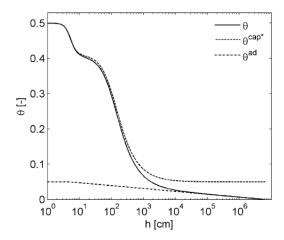


Figure 59 Typical bimodal PDI soil water retention function. The capillary part is here expressed as  $\theta^{cap^*} = \theta^{cap} + \theta_{r}$ . Thus  $\theta^{cap^*}$  resembles the classic soil water retention function with residual water content.

## C.2 CONDUCTIVITY FUNCTIONS

This section describes the conductivity functions.

#### C.2.1 GENERAL

To be valid for the complete moisture range, the liquid hydraulic conductivity model is given by a sum of capillary and film conductivity as shown in Equation 22 (Peters, 2013):

$$K = K_s \left[ (1 - \omega) K_{rel}^{cap} \left( S^{cap} \right) + \omega K_{rel}^{film} \left( S^{cap} \right) \right]$$
 Equation 22

Where  $K_s$  [cm/d] is the saturated liquid conductivity and  $K_{rel}^{cap}$   $\left[-\right]$  and  $K_{rel}^{ad}$   $\left[-\right]$  are relative conductivities for capillary and film flow.

### C.2.2 CAPILLARY CONDUCTIVITY

Relative conductivity for capillary flow is described by the pore bundle model of Mualem. The Mualem model for the capillary retention function is given by Equation 23:

$$K_{rel}^{cap}\left(S^{cap}\right) = \left(S^{cap}\right)^{\tau} \left[ \frac{\int_{0}^{S^{cap}} \frac{1}{h} dS^{cap^*}}{\int_{0}^{1} \frac{1}{h} dS^{cap^*}} \right]^{2}$$

**Equation 23** 

Where  $\tau$  [-] is the tortuosity and connectivity parameter and  $S^{cap^*}$  is a dummy variable of integration. Except for the unconstrained van Genuchten variants there exist analytical solution for all above mentioned soil water retention functions.

#### C.2.2.1 ANALYTICAL SOLUTIONS FOR UNSCALED CAPILLARY RETENTION FUNCTIONS.

For the unscaled capillary retention functions  $S^{cap} = \Gamma$ . In these cases the analytical solutions are given by Equation 24:

$$K_{rel}^{cap} = \left(S^{cap}\right)^{\tau} \left[1 - \left(1 - \left(S^{cap}\right)^{1/m}\right)^{m}\right]^{2}$$
 Equation 24

for the constrained van Genuchten function (Equation 25),

$$K_{rel}^{cap} = \left(S^{cap}\right)^{\mathsf{T}} \left[\frac{1}{2} \mathit{erfc} \left[\mathit{erfc}^{-1} - \left(2S^{cap}\right) + \frac{\sigma}{\sqrt{2}}\right]\right]^{2}$$
 Equation 25

for the Kosugi function (Equation 26),

$$K_{rel}^{cap} = \left(\sum\nolimits_{i = 1}^k {{w_i}{S_i^{cap}}} \right)^{\tau} {\left[ {1 - \frac{{\sum\nolimits_{i = 1}^2 {{w_i}{\alpha _i}{{\left( {1 - {{\left( {S_i^{cap}} \right)}^{{1/{m_i}}}} \right)}^{{m_i}}}}}}{{\sum\nolimits_{i = 1}^2 {{w_i}{\alpha _i}} }} \right]^2}$$

**Equation 26** 

for the bimodal van Genuchten function, and (Equation 27)

$$K_{rel}^{cap} = \left(\sum\nolimits_{i=1}^{k} w_{i} S_{i}^{cap}\right)^{\mathsf{T}} \left[ \frac{\sum\nolimits_{i=1}^{2} w_{i} \frac{e^{\sigma_{i}^{2}/2}}{2h_{m,i}} - \sum\nolimits_{i=1}^{2} w_{i} \frac{e^{\sigma_{i}^{2}/2}}{2h_{m,i}} erf \left[erfc^{-1}\left(2\varGamma_{i}\right) + \frac{\sigma_{i}}{\sqrt{2}}\right] \right]^{2} \\ 2\sum\nolimits_{i=1}^{2} w_{i} \frac{e^{\sigma_{i}^{2}/2}}{2h_{m,i}}$$

**Equation 27** 

for the bimodal Kosugi function.

#### C.2.2.2 ANALYTICAL SOLUTIONS FOR SCALED CAPILLARY RETENTION FUNCTIONS.

For the scaled capillary retention functions, the Mualem model can be written as (Peters, 2014) shown in Equation 28:

$$K_{rel}^{cap}\left(S^{cap}\right) = \left(S^{cap}\right)^{\tau} \left[ \frac{\int_{\Gamma_0}^{\Gamma} \frac{1}{h} d\Gamma^*}{\int_{\Gamma_0}^{1} \frac{1}{h} d\Gamma^*} \right]^2$$

**Equation 28** 

where and  $\Gamma^*$  is a dummy variable of integration. This leads to the following general solution:

$$K_{rel}^{cap}\left(S^{cap}\right) = \left(S^{cap}\right)^{\tau} \left[\frac{F\left(\Gamma\right) - F\left(\Gamma_{0}\right)}{F\left(1\right) - F\left(\Gamma_{0}\right)}\right]^{2}$$
 Equation 29

where  $F(\Gamma)$  is the solution of the indefinite integral  $\int \frac{1}{h} d\Gamma \times F(\Gamma)$  for the unimodal constrained van Genuchten and for the unimodal Kosugi function are given by:

$$F\!\left(\Gamma\right)\!=\!-\alpha\!\left(1\!-\!\Gamma^{1/m}\right)^{\!m}$$
 Equation 30

and

$$F\!\left(\Gamma\right)\!=\!-\frac{e^{\sigma^{2}/2}}{2h_{_{\!m}}}er\!f\!\left[er\!f\!c^{-1}\!\left(2\Gamma\right)\!+\!\frac{\sigma}{\sqrt{2}}\right]$$
 Equation 31

where  $erfc^{-1}$  is the inverse of the complementary error function. For the bimodal van Genuchten and Kosugi functions (Durner, 1994 and Romano et al., 2011) F(T) is given by:

$$F\!\left(\varGamma\right)\!=\!-\!\sum\nolimits_{i=1}^{2}w_{i}\alpha_{i}\!\left(1\!-\!\varGamma_{i}^{1/m_{i}}\right)^{m_{i}}$$
 Equation 32

and

$$F(\Gamma) = -\sum_{i=1}^{2} w_i \frac{e^{\sigma^2/2}}{2h_{m,i}} erf\left[erfc^{-1}(2\Gamma_i) + \frac{\sigma_i}{\sqrt{2}}\right]$$
 Equation 33

Equation 29 through Equation 33 yield the following solutions for the capillary conductivity function:

$$K_{rel}^{cap} = \left(S^{cap}\right)^{\tau} \left[1 - \left(\frac{1 - \Gamma^{1/m}}{1 - \Gamma_0^{1/m}}\right)^m\right]^2$$

**Equation 34** 

for the basic van Genuchten function,

$$K_{rel}^{cap} = \left(S^{cap}\right)^{\mathsf{T}} \left[ \frac{F_0 - erf\left(erfc^{-1}\left(2\varGamma\right) + \frac{\sigma}{\sqrt{2}}\right)}{1 + F_0} \right]^2$$

**Equation 35** 

with

$$F_{\scriptscriptstyle 0} = erf \left[ erfc^{-1} \left( 2 \varGamma_{\scriptscriptstyle 0} \right) + \frac{\sigma}{\sqrt{2}} \right]$$

**Equation 36** 

for the basic Kosugi function,

$$K_{rel}^{cap} = \left(\sum\nolimits_{i = 1}^k {{w_i}{S_i^{cap}}} \right)^{\! \top} \! \left[ 1 - \frac{{\sum\nolimits_{i = 1}^2 {{w_i}{\alpha _i}{{\left( {1 - \Gamma _i^{1/m_i}} \right)}^{{m_i}}}} }}{{\sum\nolimits_{i = 1}^2 {{w_i}{\alpha _i}{{\left( {1 - \Gamma _{0,i}^{1/m_i}} \right)}^{{m_i}}}} }} \right]^2$$

Equation 37

for the bimodal van Genuchten function and

$$K_{rel}^{cap} = \left(\sum_{i=1}^{k} 2_{i} S_{i}^{cap}\right)^{\mathsf{T}} \left[ F_{0} - \sum_{i=1}^{2} 2_{i} \frac{e^{\sigma_{i}^{2}/2}}{2h_{m,i}} erf \left[ erfc^{-l} \left( 2\Gamma_{i} + \frac{\sigma_{i}}{\sqrt{2}} \right) \right] \right]^{2} \sum_{i=1}^{2} w_{i} \frac{e^{\sigma_{i}^{2}/2}}{2h_{m,i}} + F_{0}$$

**Equation 38** 

with

$$F_{0} = \sum_{i=1}^{2} w_{i} \frac{e^{\sigma_{i}^{2}/2}}{2h_{m,i}} erf \left[ erfc^{-1} (2\Gamma_{0}) + \frac{\sigma_{i}}{\sqrt{2}} \right]$$

**Equation 39** 

For the bimodal Kosugi function.

NOTE: For  $\Gamma_0 = 0$ , Equation 35 through Equation 39 reduce to Equation 24 through Equation 27. In cases of using the unconstrained uni- or bimodal van Genuchten or Fredlund and Xing functions, the capillary bundle model of Mualem (Equation 28) is solved numerically.

### C.2.3 FILM CONDUCTIVITY

The relative conductivity for water flow in films is given by Equation 40 (Peters, 2013):

$$K_{\mathit{rel}}^{\mathit{film}} = \left(\frac{h_0}{h_a}\right)^{a\left(1 - S^{\mathit{ad}}\right)}$$

**Equation 40** 

where a [–] is the slope on the log-log scale, which might be fixed to –1.5 (Tokunaga, 2009; Peters, 2013).

### C.2.4 PREDICTION OF ISOTHERMAL VAPOR CONDUCTIVITY

SHYPFIT2.0 allows optional to ad isothermal vapor conductivity to liquid hydraulic conductivity. In that case total hydraulic conductivity is given by Equation 41:

$$K = K_s \left[ (1 - \omega) K_{rel}^{cap} \left( S^{cap} \right) + \omega K_{rel}^{film} \left( S^{ad} \right) \right] + K^{vap}$$
 Equation 41

The isothermal vapor conductivity  $K^{vap}$  is calculated according to Saito et al. (2006) as shown in Equation 42:

$$K^{vap} = rac{
ho_{sv}}{
ho_{w}} D rac{Mg}{RT} H_{r}$$
 Equation 42

Where  $\rho_{sv}$  [kg/m<sup>-3</sup>] and  $\rho_{w}$  [kg/m<sup>-3</sup>] ( $\rho_{w}$  = 1000 kg/m<sup>-3</sup>) are the saturated vapor density and the liquid density of water, M [kg/mol<sup>-1</sup>] (M = 0.018015 kg mol<sup>-1</sup>) is the molecular weight of water, g [m s<sup>-2</sup>] (g = 9.81 m s<sup>-2</sup>) is the gravitational acceleration, R [j mol<sup>-1</sup> Kg<sup>-1</sup>] (R = 8.314 J mol<sup>-1</sup> Kg<sup>-1</sup>) is the universal gas constant, T [K] is the absolute temperature, D [m<sup>2</sup> s<sup>-1</sup>] is the vapor diffusivity and  $H_r$  [–] is the relative humidity. D is dependent on water content and is calculated according to Saito et al. (2006) using Equation 43:

$$D = \xi \theta_a D_a$$
 Equation 43

Where  $\Theta_a$  [–] is the volumetric air content, for simplicity given by: theta\_a = theta\_s – theta,  $D_a$  [m<sub>2</sub> s<sub>-1</sub>] is the diffusivity of water vapor in air and  $\xi$  [–] is the tortuosity factor for gas transport, calculated according to Millington and Quirk (1961) shown in Equation 44:

$$\xi = \frac{\theta_a^{7/3}}{\theta_s^2}$$

Equation 44

 $D_a$  and  $p_{sv}$  are dependent on temperature (Equation 45):

$$D_a = 2.14 \times 10^{-5} \left( \frac{T}{273.15} \right)^2$$

**Equation 45** 

and (Equation 46)

$$\rho_{sv} = 10^{-3} \exp\left[31.3716 - \frac{6014.79}{T} - 7.92495 \times 10^{-3}T\right]T^{-1}$$

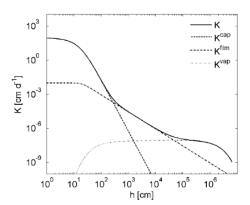
**Equation 46** 

 $H_{c}$  is calculated with the Kelvin equation (Equation 46):

$$H_{r} = exp \bigg( \frac{hMg}{RT} \bigg)$$

**Equation 47** 

Figure 60 shows total hydraulic conductivity and the single parts for an unimodal and bimodal capillary retention function.



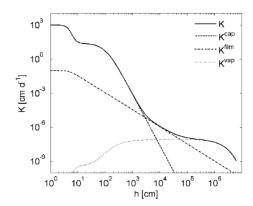


Figure 60 Total hydraulic conductivity for unimodal (left) and bimodal (right) capillary retention function

# **C.3 CAPACITY FUNCTIONS**

The soil water capacity function is defined as in Equation 48:

$$C(h) = \frac{d\theta}{dh}$$

Equation 48

The general form of the PDI capacity function is calculated with Equation 49

$$C(h) = (\theta_s - \theta_r) \frac{dS^{cap}}{dh} + \theta_r \frac{dS^{ad}}{dh} = \frac{\theta_s - \theta_r}{1 - \Gamma_0} \frac{d\Gamma}{dh} + \theta_r \frac{dS^{ad}}{dh}$$

Equation 49

where the derivative of the adsorptive saturation is given by using Equation 50:

$$\frac{dS^{ad}}{dh} = \frac{1}{h \ln(10)(x_a - x_0)} \left[ 1 - \frac{exp\left(\frac{x_a - x}{b}\right)}{1 + exp\left(\frac{x_a - x}{b}\right)} \right]$$

Equation 50

The difference between the derivatives of the scaled and unscaled capillary saturation functions is only the denominator  $1 - \Gamma_0$  which is 1 for the unscaled function. Therefore, the derivatives are given for the unscaled functions. The derivatives are (Equation 51):

$$\frac{d\Gamma}{dh} = -\alpha nm(\alpha h)^{n-1} \left[1 + (\alpha h)^{n}\right]^{-(m+1)}$$

Equation 51

for the unimodal van Genuchten function (Equation 52),

$$\frac{d\Gamma}{dh} = \frac{1}{\sqrt{2\pi\sigma h}} exp \left[ -\frac{\left[ In \left( \frac{h}{h_m} \right) \right]^2}{2\sigma^2} \right]$$

Equation 52

for the unimodal Kosugi function (Equation 53),

$$\frac{d\Gamma}{dh} = \frac{mn(\alpha h)^n \left\{ ln \left[ (\alpha h)^n + e \right] \right\}^{-m-1}}{h(\alpha h)^n + eh}$$

Equation 53

For the basic Fredlund and Xing function and simply (Equation 54)

$$\frac{d\Gamma}{dh} = \sum_{i=1}^{2} w_i \frac{d\Gamma_i}{dh}$$

**Equation 54** 

for the bimodal functions.

## C.4 OTHER SOIL HYDRAULIC FUNCTIONS

The hydraulic functions summarized in Section C.1encompass most of the commonly used soil hydraulic functions (such as the original van Genuchten, Kosugi and Durner functions) and extend them to account for water retention and conductivity in incompletely filled pores as well as for isothermal vapor conductivity. Sometimes other models which are not part of the PDI model family are required such as the Brooks and Corey (1964) model or the model from Fredlund and Xing (1994). These two models are outlined here.

### C.4.1 BROOKS AND COREY FUNCTION

The Brooks and Corey retention function is given by Equation 55:

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

**Equation 55** 

where  $\alpha$  [1/cm] is the inverse of the air entry value,  $\lambda$  [-] is the pore size distribution index and  $S_e$  is the effective saturation given by  $S_e = (\Theta - \Theta_r) / (\Theta_s - \Theta_r)$  with  $\Theta_s$  and  $\Theta_r$  are saturated and residual water contents.

Based on similar capillary bundle considerations as the Mualem model, the combination of the Brooks & Corey retention function with the Burdine conductivity model (Burdine, 1953) gives (Brooks and Corey, 1964) Equation 56:

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 [–], which is regarded as fitting parameter.

The capacity relation for the Brooks and Corey function is given by Equation 57:

$$C\!\left(h\right)\!=\! \left\{ \begin{smallmatrix} (\theta_s-\theta_r)\frac{\lambda}{h}\!\left(\alpha h\right)^{-\lambda} & \text{ for } h\!>\!\alpha^{-1} \\ 0 & \text{ for } h\!\leq\!\alpha^{-1} \end{smallmatrix} \right.$$

Equation 57

### C.4.2 ORIGINAL FREDLUND AND XING MODEL

The Fredlund and Xing (1994) soil water retention model accounts for zero water content at oven dryness by Equation 58:

$$\theta(h) = \theta_{sX}(h)\Gamma(h)$$

Equation 58

with Equation 59

$$\Gamma(h) = \left\{ In \left[ e + \left(\alpha h\right)^n \right] \right\}^{-m}$$

**Equation 59** 

and Equation 60

$$X(h) = 1 - \frac{In(1 + h/h_r)}{In(1 + h_0/h_r)}$$

Equation 60

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where  $\alpha$ , n, m, and h, are curve shape parameters and e is the Euler number. For the Fredlund and Xing retention model there exists no analytical solution for the Mualem capillary bundle model. Therefore, Equation 28 is solved numerically.

The capacity function for the Fredlund and Xing retention model is Equation 61:

$$C(h) = \frac{d_X}{dh}\Gamma + \frac{d\Gamma}{dh}X$$

Equation 61

where Equation 62

$$\frac{d_{X}}{dh} = \frac{1}{\left(h + h_{r}\right) ln \left(\frac{h_{r}}{h_{r} - h_{0}}\right)}$$

**Equation 62** 

and Equation 63

$$-\frac{d\Gamma}{dh} = \frac{mn(\alpha h)^n \left\{ ln \left[ (\alpha h)^n + e \right] \right\}^{-m-1}}{h(\alpha h)^n + eh}$$

Equation 63

Table 15 Summary of All Implemented Model Combinations In SHYPFIT2.0

Basic	Mod	Scal	Ads	Code	1	2	3	4	5	6	7	8	9	10	11	12	13	14
vG	uni	no	no	1100	α	n	$\theta_r$	$\theta_{s}$	$K_s$	τ								
vG	uni	yes	no	1110	α	n	_	$\theta_{s}$	$K_s$	τ	$h_0$							
vG	uni	no	yes	1101	α	n	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а					
vG	uni	yes	yes	1111	α	n	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	a					
Kos	uni	no	no	2100	$h_{\scriptscriptstyle m}$	$\sigma$	$\theta_r$	$\theta_{s}$	$K_s$	τ								
Kos	uni	yes	no	2110	$h_m$	σ	_	$\theta_{s}$	$K_s$	τ	$h_o$							
Kos	uni	no	yes	2101	$h_m$	σ	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а					
Kos	uni	yes	yes	2111	$h_{\scriptscriptstyle m}$	σ	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а					
vG	bi	no	no	1200	$\alpha$	n	$\theta_r$	$\theta_{s}$	$K_s$	τ	_	_	_	$\alpha_2$	$\sigma_{\!\scriptscriptstyle 2}$	$W_c$		
vG	bi	yes	no	1210	α	n	_	$\theta_{s}$	$K_s$	τ	$h_0$	_	_	$\alpha_2$	$\sigma_{2}$	$W_c$		
vG	bi	no	yes	1201	α	n	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а	$\alpha_2$	$\sigma_{2}$	$W_c$		
vG	bi	yes	yes	1211	α	n	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а	$\alpha_2$	$\sigma_{2}$	$w_c$		

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Table 15 Summary of All Implemented Model Combinations In SHYPFIT2.0 (continued)

Basic	Mod	Scal	Ads	Code	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Kos	bi	no	no	2200	$h_m$	$\sigma$	$\theta_r$	$\theta_{s}$	$K_s$	τ	_	_	_	$h_{m,2}$	$\sigma_{\!\scriptscriptstyle 2}$	$w_c$		
Kos	bi	yes	no	2210	$h_m$	σ	_	$\theta_{s}$	$K_s$	τ	$h_0$	_	_	$h_{m,2}$	$\sigma_{\!\scriptscriptstyle 2}$	$W_c$		
Kos	bi	no	yes	2201	$h_m$	σ	$\omega$	$\theta_{s}$	$K_s$	$\tau$	$h_0$	$\omega$	а	$h_{m,2}$	$\sigma_{2}$	$W_c$		
Kos	bi	yes	yes	2211	$h_{\scriptscriptstyle m}$	$\sigma$	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	a	$h_{m,2}$	$\sigma_{2}$	$W_c$		
vGm	uni	no	no	3100	α	n	$\theta_r$	$\theta_{s}$	$K_s$	τ	_	_	_	m				
vGm	uni	yes	no	3110	α	n	_	$\theta_{s}$	$K_s$	τ	$h_0$	_	_	m				
vGm	uni	no	yes	3101	α	n	$\omega$	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а	m				
vGm	uni	yes	yes	3111	α	n	ω	$\theta_{s}$	$K_s$	τ	$h_0$	ω	a	m				
vGm	bi	no	no	1200	α	n	$\theta_r$	$\theta_{s}$	$K_s$	τ	_	_	_	$\alpha_2$	$n_2$	$w_c$	m	$m_2$
vGm	bi	yes	no	1210	α	n	_	$\theta_{s}$	$K_s$	τ	$h_0$	_	_	$\alpha_2$	$n_2$	$W_c$	m	$m_2$
vGm	bi	no	yes	1201	α	n	ω	$\theta_s$	$K_s$	τ	$h_0$	ω	а	$\alpha_2$	$n_2$	$W_c$	m	$m_2$
vGm	bi	yes	yes	1211	α	n	ω	$\theta_{s}$	$K_s$	τ	$h_o$	ω	a	$\alpha_2$	$n_2$	$w_c$	m	$m_2$
BC// Bur				4000	$h_a$	λ	$\theta_r$	$\theta_{s}$	$K_s$	τ								
FX	uni			5000	α	n	$h_r$	$\theta_{s}$	$K_s$	τ	$h_0$	m						
FX	uni	yes	yes	5111	α	n	$h_r$	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а	m				
FX	uni	yes	yes	5211	α	n	$h_r$	$\theta_{s}$	$K_s$	τ	$h_0$	ω	а	$\alpha_2$	$n_2$	$w_c$	m	$m_2$

a Basic-Basic functions

Kos-Kosugi

vGm-van Genuchten unconstrained

Mod-Modality

uni-unimodal

bi-bimodal

Scal-Scaling

Ads-Adsorption

Information in the preceding list are either considered or not considered. If Ads is considered, film conductivity is considered as well.

NOTE: The greyed out models are not directly implemeted in LABROS SoilView-Analysis.

vG-van Genuchten constrained

### C.5 PARAMETER ESTIMATION

The following section describes the parameter estimation.

### C.5.1 DEFINITION OF OBJECTIVE FUNCTION

The parametric models for  $\theta(h)$  and K(h) are fitted simultaneously to the data points. This is essential as distinct parameters (e.g.,  $\alpha$  and n for the van Genuchten/Mualem model) influence the shape of both functions. The fitting is accomplished by a nonlinear regression algorithm by minimizing the sum of weighted squared residuals between model prediction and data pairs:

$$\Phi(b) = \omega_{\theta} \sum_{i=1}^{r} \omega_{\theta,i} \left[ \overline{\theta}_{l} - \hat{\theta}_{i}(b) \right]^{2} + \omega_{K} \sum_{i=1}^{r} \omega_{K,i} \left[ K_{i} - \widehat{K}_{i}(b) \right]^{2}$$
Equation 64

where r and k are the number of data pairs for the retention and the conductivity function, respectively,  $w_{\theta}$  and  $w_{K}$  are the class weights of the water content data and conductivity data,  $w_{\theta,i}$  and  $w_{K,i}$  are the weights of the individual data points, and  $\bar{\theta}_{i},\hat{\theta}_{i}(b),K_{i}$ , and  $K_{i}(b)$  are the measured and model predicted values, respectively and b is the parameter vector. In SHYPFIT2.0 either the combination of  $\theta(h)$  and K(h) models or only one of them can be fitted to the measured data. In the latter case the first or second part of Equation 64 vanishes.

The parameter estimation procedure must guarantee that the best parameter combination for the appropriate model combination is found (i.e., the global minimum in the multidimensional parameter space must be determined). Often local estimation algorithms such as the Levenberg-Marquardt algorithm (Marquardt, 1963) are used for parameter estimation. However, especially for complex models with many degrees of freedom these algorithms fail to find the optimal parameter vector so that the outcome of these algorithms largely depends on the initial guesses. Therefore, SHYPFIT2.0 uses the shuffled complex evolution algorithm (SCE) (Duan et al., 1992), which is a global parameter estimation algorithms.

One crucial part is the choice of the correct boundaries for the parameters. In SHYPFIT2.0 the boundaries of the parameters for each model combination have default values, which might be changed by the user if necessary. The predefined boundaries are chosen in a way, which shall guarantee high flexibility on the one hand and physical consistency on the other hand. To guarantee both for the parameter of the Mualem conductivity model (Equation 28), the lower allowed boundary of tau can be expressed as a function of the pore-size distribution parameters of the retention function as described by Peters et al. (2011). For the unscaled uni- and bimodal van Genuchten retention functions, the lower allowed value is given by:  $\tau_{min} = 1 - 2/m$  and  $\tau_{min} = 1 - 2_{min} |1/_{mi}|$ , respectively.

### C.5.2 INTEGRAL VERSUS CLASSIC FIT

For Equation 64, the predicted water contents,  $\theta_i$ , are either calculated in a standard manner as the point water contents at pressure head  $h_i$ , (classic method), or as the mean water content of the column, calculated as the integral of the water content distribution over the soil column divided by its height (integral method).

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In the case that the measured water contents and pressure heads are regarded as point measurements in the soil they are treated as simple points of the fitted soil water retention function. This scheme is called the classic method.

In the case of hydrostatic column experiments or when evaporation experiments are conducted and the water contents are measured as mean water contents in the whole soil column with a scale, Peters and Durner (2006, 2008a) introduced the so called integral method. This is done since the assumption that the water content is spread out linear over the column is not always fulfilled in coarse pored or structured soil. Effectively, the measured mean water content of the column is the integral of the water content distribution over the whole column divided by the volume of the column. With the assumption of hydraulic equilibrium (for hydrostatic experiments) or quasi equilibrium (for the early stage of evaporation experiments (Peters and Durner, 2008a)) this is in the one-dimensional case the same as the integral of the retention function over the matric heads from the lower boundary of the column to the upper boundary divided by the height of the column. Therefore, we have to replace in Equation 64 the model predicted point water content  $\hat{\theta}_i(b)$  by the model predicted mean water content:

$$\hat{\theta}_{i}(b) = \frac{1}{L} \int_{h_{b,i}}^{h_{ub,i}} \hat{\theta}(b,h) dh$$

Equation 65

where L [cm] is the column height, and  $h_{ub,i}$  and  $h_{lb,i}$  indicate the upper boundary and lower boundary suctions for each equilibrium state. If the option integral fit is selected, the column length must be given. In this case, SHYPFIT2.0 interprets the measured suction as the suction in the soil center and calculates the  $h_{ub}$  and  $h_{lb}$  by assuming hydrostatic equilibrium, (i.e.,  $h_{ub} = h + L/2$  and  $h_{lb} = h + L/2$ ).

#### C.5.3 WEIGHING SCHEMES

Since the objective function  $\Phi(b)$  (Equation 64) involves data of different types with different measurement frequency, the result of the optimization will likely be affected by the weights of the data (Simunek and Hopmans, 2002). Therefore, the user can choose between three different weighting schemes.

In the first scheme the user is fully responsible for data weighting. Each data pair will get a single weight. No extra calculations will be carried out. If the user has prior knowledge about measurement errors, this scheme might be used. For normally distributed uncorrelated measurement errors with zero mean, the single weights can be set to the reciprocal of the variance of the measurement error. This is in accordance with the maximum likelihood principle for the method of least squares (Omlin and Reichert, 1999). In this scheme  $w_{\theta}$  and  $w_{\kappa}$  are both set to unity and  $w_{\theta i}$  and  $\omega_{\kappa j}$  and  $\omega_{\kappa j}$  and  $\omega_{\kappa j}$  are the variances of single the measurement errors.

In the second scheme the weights are first normalized by a factor for the data type and second by a factor for the data frequency as suggested by Peters and Durner (2008a). To account for the different measurement frequency, the individual weights,  $\omega_{\theta,i}$  and  $\omega_{K,i}$  are

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chosen such that the combined data within every  $\log_{10}(h\,[\mathrm{cm}]) = \mathrm{pF}$  increment have the same weight (i.e., the weight for a certain data point is proportional to its distance to the neighboring point on the pF scale). To account additionally for the different data types, the weights for the data classes are calculated by  $\omega_{\theta} = 1/(\theta_{max} - \theta_{min})$  and  $\omega_{\kappa} = 1/(\log_{10}(K_{max}) - \log_{10}(K_{min}))$  where  $\theta_{max}$ ,  $\theta_{min}$ ,  $K_{max}$ , and  $K_{min}$  are the maximum and minimum values of the data sets to which the models are fitted.

The third scheme is similar to the second scheme regarding the weights on the pF scale, (i.e.,  $\omega_{\theta i}$  and  $\omega_{K,i}$ ). The weights for the different classes (i.e.,  $\omega_{\theta}$  and  $\omega_{K}$ ) are in this scheme given by the user. Schelle et al. (2010), for example, set  $\omega_{\theta}$  and  $\omega_{K}$  to 1 and 0.001, respectively, and found good results. The last two weighting schemes are only applicable in the case that no repetitions are measured, because then different data pairs may have similar or equal pF values, so that several data points will get weights of or close to 0.

## C.6 POSTPROCESSING

The following section describes postprocessing.

### C.6.1 DIAGNOSTIC VARIABLES

The first measure to evaluate the performance of the fitted model is the objective function values at their estimated minimum,  $\Phi_{min}$ , in this case the weighted sum of squared residuals.

A more descriptive measure, giving the mean deviation between model and data is the root mean square error, RMSE (Equation 66):

$$\mathsf{RMSE} = \sqrt{\frac{1}{r} \sum_{i=1}^{r} \left[ y_i - \hat{y}_i \right]^2}$$

**Equation 66** 

where  $y_i$  and  $\hat{y}_i$  are measured and model predicted quantities (i.e., water contents or hydraulic conductivities,  $\log_{10}(K)$ ). For a sound representation of the data by the model, the values of RMSE should be close to the measurement error.

The Nash-Sutcliffe index (Nash and Sutcliffe, 1970) and coefficient of determination are calculated for both data types. The Nash-Sutcliffe index is given by Equation 67:

$$E = 1 - \frac{\sum_{1}^{r} [y_{i} - \hat{y}_{i}]^{2}}{\sum_{1}^{r} [y_{i} - \overline{y}_{i}]^{2}}$$

Equation 67

where  $\overline{y}_i$  is the mean measured quantity.

The coefficient of determination  $(r^2)$  is given by Equation 68:

$$r^{2} = 1 - \frac{\sum_{1}^{r} \left[ y_{i} - \overline{y}_{i} \right] \left[ \hat{y}_{i} - \overline{\hat{y}}_{i} \right]}{\sqrt{\sum_{1}^{r} \left[ y_{i} - \overline{y}_{i} \right]^{2} \left[ \hat{y}_{i} - \overline{\hat{y}}_{i} \right]^{2}}}$$

Equation 68

To account for the different number of adjustable parameters when comparing different models fitted to the same data, SHYPFIT2.0 also calculates the Akaike Information Criterion, AIC = 2(L + k) (Akaike, 1974), where L is the likelihood function and k is the number of fitting parameters. In a least squares estimation and with  $N(0,\sigma^2)$  distributed residuals the information criterion, AIC, can be expressed in the form (Equation 69) as described by Ye et al. (2008):

$$AIC = nln(\Phi_{min}/n) + 2k$$
 Equation 69

where n is the number of measured data and k is the number of adjustable parameters. If the number of measurements, n, is small in comparison to k, the original form of AIC should be extended by a correction term that accounts for small values for n/k (Hurvich and Tsai, 1989), leading to the extended information criterion (Equation 70):

$$\mathsf{AICc} = nl\mathsf{n} \Big( \varPhi_{\scriptscriptstyle min} \ / \ n \Big) + 2k + \left( \frac{2k \big(k+1\big)}{n-k-1} \right)$$
 Equation 70

The first term penalizes a poor fit, the second term the number of parameters and the third term is the correction term for small values of n/k. If n/k becomes large, the last term becomes negligible and the AICc converges to AIC.

Since sometimes other information criteria are suggested as well, SHYPFIT2.0 calculates also the BIC and KIC for model selection. These two are given for least square estimations (Equation 71) as follows (Ye et al., 2008):

$$\mathsf{BIC} = n!\mathsf{n}\big(\Phi_{\scriptscriptstyle min} \,/\, n\big) + k\, ln\big(n\big)$$
 Equation 71

and Equation 72

$$\mathsf{KIC} = (n-k)\mathsf{In}\big(\Phi_{\min} \ / \ n\big) + k\mathsf{In}\big(J^{\mathsf{\scriptscriptstyle T}} wJ\big)$$
 Equation 72

Where  $|J^T\omega J|$  is the determinant of the Fisher information matrix. J is the Jacobian or sensitivity matrix with elements  $J_{i,j}=\partial\hat{z}_i/\partial b_i$  where  $\hat{z}_i$  is the model prediction at point i and  $b_j$  is the j-th parameter. The superscript T indicates the transpose of the matrix and  $\omega$  is the weighting matrix.

### C.6.2 UNCERTAINTY ANALYSIS

The following sections describe uncertainty analysis.

#### C.6.2.1 PARAMETER UNCERTAINTIES

In order to evaluate the uncertainties of the estimated parameters a linear approximation of the covariance matrix of the estimated parameters,  $C_p$  is calculated as shown in Equation 73 (Omlin and Reichert, 1999):

$$C_p pprox rac{\Phi_{ extit{min}}}{n-k} ig(J^{^T}wJig)^{^{-1}}$$
 Equation 73

The linear approximation leads to a confidence interval for the *i-th* estimated parameter  $\hat{b}_i$  by Equation 74:

$$\hat{b}_i \pm \sqrt{C_{\rho_{i,i}}} \times t_{n-k,\alpha/2}$$

Equation 74

where  $t_{n-k,\omega/2}$  is the upper  $\alpha/2$  quantile of the students t-distribution with n-k degrees of freedom.  $\alpha$  is set to 0.05 leading to the 95% confidence interval for the parameters.

### **C.6.2.2 FUNCTION UNCERTAINTIES**

The uncertainties for the  $\theta(h)$  and K(h) functions are determined by calculating the covariance of the model response (Equation 75),  $C_a$ :

$$C_z pprox J^T C_{
ho} J$$
 Equation 75

where the J is the Jacobian or sensitivity matrix with elements  $J_{ij} = \partial \hat{z}_i / \partial b_i$  where  $\hat{z}_i$  is the model prediction at point i and  $b_j$  is the jth parameter. The confidence interval for the model output is given by Equation 76:

$$\widehat{y_i} \pm \sqrt{C_{z_{i,i}}} \times t_{n-k,\alpha/2} \hspace{1cm} \text{Equation 76}$$

where  $\hat{\mathbf{y}}_i$  is the model output  $\hat{\boldsymbol{\theta}}_i$  and  $\log_{10}(\widehat{K}_i)$  for the retention and conductivity function, respectively. Again,  $\alpha$  is set to 0.05 leading to the 95% confidence intervals for the functional relationships.

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